## Stability of Black Box Algorithms

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## Outline

- Background on algorithmic stability
- Part 1: hardness of testing stability ${ }^{1}$
- Part 2: stability for bagged algorithms ${ }^{2}$

Collaborators:


[^0]
## Background: algorithmic stability

Data $\left(X_{1}, Y_{1}\right), \ldots,\left(X_{n}, Y_{n}\right) \in \mathbb{R}^{d} \times \mathbb{R} \xrightarrow{\text { algorithm } \mathcal{A}}$ Fitted model $\widehat{f}$

- Can $\widehat{f}$ estimate the true model for $Y \mid X$ ?
- Is $\widehat{f}$ guaranteed to predict $Y$ with low test error?
- Is training error $\approx$ test error?
- Can we estimate how well $\widehat{f}$ predicts $Y$ from $X$ ?
more assumptions
distribution-free?


## Background: algorithmic stability

Concentration / consistency: $\widehat{f} \approx \widehat{f}^{\prime}$ if we resample entire data set
Stability: $\widehat{f} \approx \widehat{f}^{\prime}$ if we resample small fraction of data set

## Background: algorithmic stability

## Definition

$\mathcal{A}$ is $(\epsilon, \delta)$-stable with respect to distribution $P$ \& sample size $n$ if

$$
\mathbb{P}_{P}\left\{\left|\widehat{f}\left(X_{n+1}\right)-\widehat{f}^{i}\left(X_{n+1}\right)\right|>\epsilon\right\} \leq \delta \text { for }\left(X_{j}, Y_{j}\right) \stackrel{\text { iid }}{\sim} P
$$

$\mathcal{A}$ trained on $\left\{\left(X_{j}, Y_{j}\right) ; j \in[n]\right\} \quad \mathcal{A}$ trained on $\left\{\left(X_{j}, Y_{j}\right): j \in[n] \backslash i\right\}$

Notes:

- We assume $\mathcal{A}$ treats training data symmetrically

$$
\mathcal{A}\left(\left(X_{1}, Y_{1}\right), \ldots,\left(X_{n}, Y_{n}\right)\right)=\mathcal{A}\left(\left(X_{\sigma(1)}, Y_{\sigma(1)}\right), \ldots,\left(X_{\sigma(n)}, Y_{\sigma(n)}\right)\right)
$$

- Framework \& results allow for a randomized $\mathcal{A}$


## Motivation for algorithmic stability

Stability has implications for:

- Generalization [Bousquet \& Elisseeff 2002; Elisseeff et al 2005]
- Learnability [Shalev-Shwartz et al 2010]
- Predictive inference
[Steinberger \& Leeb 2018; B., Candès, Ramdas, Tibshirani 2021]


## Motivation for algorithmic stability - generalization

After training a model $\widehat{f}=\mathcal{A}\left(\left(X_{i}, Y_{i}\right)_{i \in[n]}\right) \ldots$

- Want to estimate $L(\widehat{f})$, where $L(f)=\mathbb{E}[\ell(f(X), Y)]$
- Leave-one-out estimate $L_{\text {LOO }}(\widehat{f})=\frac{1}{n} \sum_{i=1}^{n} \ell\left(\widehat{f}{ }^{i}\left(X_{i}\right), Y_{i}\right)$


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Stability leads to generalization: [Bousquet \& Elisseeff 2002]

- If $\ell$ is bounded and $\mathcal{A}$ satisfies

$$
\mathbb{E}\left[\left|\ell\left(\widehat{f}\left(X_{n+1}\right), Y_{n+1}\right)-\ell\left(\widehat{f}{ }^{i}\left(X_{n+1}\right), Y_{n+1}\right)\right|\right] \leq \epsilon
$$

then

$$
L(\widehat{f}) \leq L_{\mathrm{LOO}}(\widehat{f})+\mathcal{O}_{P}\left(n^{-1 / 2}+\epsilon^{1 / 2}\right) .
$$

## Motivation for algorithmic stability - predictive inference

## Definition: distribution-free predictive set

A map from data $\left(X_{i}, Y_{i}\right)_{i \in[n]}$ to a prediction band $\widehat{C}_{n}$ s.t.

$$
\mathbb{P}_{\left(X_{i}, Y_{i}\right)^{\text {idd }} \sim P}\left\{Y_{n+1} \in \widehat{C}_{n}\left(X_{n+1}\right)\right\} \geq 1-\alpha
$$

for every distribution $P$.

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Methods:

- Conformal prediction - high computational cost [Vovk et al 2005]
- Split conformal (i.e., holdout set) - less precise b/c split data
- Jackknife a.k.a. leave-one-out cross-validation — is it distrib.-free?


## Motivation for algorithmic stability - predictive inference

Jackknife: fix any regression algorithm $\mathcal{A}$, then compute

$$
\widehat{f}=\mathcal{A}\left(\left(X_{i}, Y_{i}\right)_{i \in[n]}\right), \quad \widehat{f} \backslash i=\mathcal{A}\left(\left(X_{j}, Y_{j}\right)_{j \in[n] \backslash\{i\}}\right)
$$

Prediction interval for $Y_{n+1}$ given $X_{n+1}=x$ :

$$
\widehat{C}_{n}(x)=\widehat{f}(x) \pm Q_{1-\alpha}\left(R_{i}\right)
$$

where $R_{i}=\left|Y_{i}-\widehat{f}{ }^{i}\left(X_{i}\right)\right|=i$ th leave-one-out residual

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Is this method distribution-free?

- No assumption-free guarantees $-\widehat{f} \& \widehat{f}^{i}$ may behave differently
- If $\mathcal{A}$ is $(\epsilon, \delta)$-stable, guarantees w/o any assumptions on $P$ [Steinberger \& Leeb 2018; B., Candès, Ramdas, Tibshirani 2021]


## Motivation for algorithmic stability

At a high level...
We want methods that are valid with no untestable assumptions

- We can't test whether $P$ satisfies distributional assumptions (e.g., parametric model / smoothness / etc)
- Some robust methods (e.g., jackknife) instead assume $\mathcal{A}$ is stable
- But, is this another untestable assumption?


## Aren't most algorithms stable?

Some algorithms are known to satisfy stability:

- Nearest neighbors:

$$
\widehat{f}(x)=\frac{1}{k} \sum_{i \in k-\mathrm{NN}(x)} Y_{i}
$$

Stable if we choose $k \ll n$

- Ridge regression:

$$
\widehat{f}=\phi\left(x ; \widehat{\beta}_{n}\right) \text { where } \widehat{\beta}_{n}=\arg \min _{\beta}\left\{\frac{1}{n} \sum_{i=1}^{n} \ell\left(Y_{i} ; \phi\left(X_{i} ; \beta\right)\right)+\lambda\|\beta\|_{2}^{2}\right\}
$$

Stable if $f$ and $\ell$ are Lipschitz

## Aren't most algorithms stable?

Exhibit A: least squares - known to be unstable if $d \approx n$


## Aren't most algorithms stable?

Exhibit B: modern ML methods - too complex to prove stability


Figure from A Survey of Deep-Learning Applications in Ultrasound: Artificial Intelligence-Powered Ultrasound for Improving Clinical Workflow, Akkus et al 2019

## Aren't most algorithms stable?

Exhibit C: some methods have instability built in

- Lasso (glmnet R package):

```
glmnet(x,y,\ldots, lambda.min.ratio = ifelse(nobs < nvars,0.01,1e-04) ,...)
```

- Highly adaptive Lasso (hal9001 R package):

SL.hal(Y,X,..., nfolds = ifelse(length(Y) $<=100,20,10$ ) , ...)

- Multiple imputation (mice \& midastouch R package):

In an old version of the code: outout <- ifelse(nobs>250,FALSE,TRUE)

## Part 1: Testing stability in the black box setting

The black box setting: we learn how $\mathcal{A}$ works by running it on data, e.g.:

- Run $\mathcal{A}$ on samples bootstrapped from available real data
- Run $\mathcal{A}$ on semisynthetic data obtained by perturbing the real data
- Run $\mathcal{A}$ on simulated data obtained by fitting a model to real data
- Etc.


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- Etc.

But, we cannot "look inside the black box" of $\mathcal{A}$ or of a fitted $\widehat{f}$ :

- Cannot compute $\sup _{\left(x^{\prime}, y^{\prime}\right)}\left|[\mathcal{A}(\mathcal{D})](x)-\left[\mathcal{A}\left(\mathcal{D} \cup\left(x^{\prime}, y^{\prime}\right)\right)\right](x)\right|$
- Cannot check if $\widehat{f}=\mathcal{A}(\mathcal{D})$ is Lipschitz
- Etc.


## Part 1: Testing stability in the black box setting

We want to construct a test $\widehat{T}=\widehat{T}_{n, \epsilon, \delta}\left(\mathcal{A}, \hat{\mathcal{D}}_{\ell}, \hat{\mathcal{D}}_{u}\right)$ that:
$\left\{\begin{array}{l}\text { Returns } 1 \text { if we are confident that }(\mathcal{A}, P, n) \text { is }(\epsilon, \delta) \text {-stable } \\ \text { Returns } 0 \text { otherwise }\end{array}\right.$

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We want to construct a test $\widehat{T}=\widehat{T}_{n, \epsilon, \delta}\left(\mathcal{A}, \stackrel{\mathcal{D}}{\ell}^{\ell}, \stackrel{\mathcal{D}}{u}^{u}\right)$ that:
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- We require $\widehat{T}$ to be a valid distribution-free test of $(\epsilon, \delta)$-stability:
$\mathbb{P}_{\nwarrow}\left\{\widehat{T}_{n, \epsilon, \delta}\left(\mathcal{A}, \mathcal{D}_{\ell}, \mathcal{D}_{u}\right)=1\right\} \leq \alpha$ for any $(\mathcal{A}, P, n)$ that is not $(\epsilon, \delta)$-stable with respect to data $\mathcal{D}_{\ell}, \mathcal{D}_{u}$ drawn i.i.d. from $P$
- We want $\widehat{T}$ to have high power for detecting stability:

$$
\mathbb{P}\left\{\widehat{T}_{n, \epsilon, \delta}\left(\mathcal{A}, \mathcal{D}_{\ell}, \mathcal{D}_{u}\right)=1\right\} \stackrel{? ? ?}{>} \alpha \text { for }(\epsilon, \delta) \text {-stable }(\mathcal{A}, P, n)
$$

## Black-box tests

## Definition: black-box test

available labeled \& unlabeled data
$\widehat{T}=\widehat{T}\left(\mathcal{A}, \stackrel{\mathcal{D}}{\ell}^{\ell}, \mathscr{\mathcal { D }}_{u}\right)$ is a black-box test if it can be defined as follows:

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- At step $r=1$, generate a new dataset (e.g., via subsampling/bootstrap/simulation)

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\left(\mathcal{D}_{\ell}^{(1)}, \mathcal{D}_{u}^{(1)}\right)=f^{(1)}\left[\mathcal{D}_{\ell}, \mathcal{D}_{u}\right]
$$

and train and evaluate the model,

$$
\widehat{f}^{(1)}=\mathcal{A}\left(\mathcal{D}_{\ell}^{(1)}\right), \quad \widehat{\mathbf{Y}}^{(1)}=\widehat{f}^{(1)}\left(\mathcal{D}_{u}^{(1)}\right)
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$$

- At step $r=2$, generate a new dataset

$$
\left(\mathcal{D}_{\ell}^{(2)}, \mathcal{D}_{u}^{(2)}\right)=f^{(2)}\left[\mathcal{D}_{\ell}, \mathcal{D}_{u}, \mathcal{D}_{\ell}^{(1)}, \mathcal{D}_{u}^{(1)}, \widehat{\mathbf{Y}}^{(1)}\right]
$$

and train and evaluate the model,

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- Repeat for $r=3,4, \ldots$


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$$
\widehat{f}^{(2)}=\mathcal{A}\left(\mathcal{D}_{\ell}^{(2)}\right), \quad \widehat{\mathbf{Y}}^{(2)}=\widehat{f}^{(2)}\left(\mathcal{D}_{u}^{(2)}\right)
$$

- Repeat for $r=3,4, \ldots$
- Finally, define $\widehat{T}=g\left[\mathcal{D}_{\ell}, \mathcal{D}_{u},\left(\mathcal{D}_{\ell}^{(r)}\right)_{r \geq 1},\left(\mathcal{D}_{u}^{(r)}\right)_{r \geq 1},\left(\widehat{\mathbf{Y}}^{(r)}\right)_{r \geq 1}\right]$.


## Binomial test

$$
\text { Let } \begin{aligned}
\kappa & =\min \left\{\frac{\left|\mathcal{D}_{\ell}\right|}{n}, \frac{\left|\mathcal{D}_{\ell}\right|+\left|\mathcal{D}_{u}\right|}{n+1}\right\} \\
& \rightsquigarrow \text { can construct }\lfloor\kappa\rfloor \text { many data sets }\left(X_{1}^{k}, Y_{1}^{k}\right), \ldots,\left(X_{n}^{k}, Y_{n}^{k}\right), X_{n+1}^{k}
\end{aligned}
$$

A simple binomial test

## Binomial test

Let $\kappa=\min \left\{\frac{\left|\mathcal{D}_{\ell}\right|}{n}, \frac{\left|\mathcal{D}_{\ell}\right|+\left|\mathcal{D}_{u}\right|}{n+1}\right\}$
$\rightsquigarrow$ can construct $\lfloor\kappa\rfloor$ many data sets $\left(X_{1}^{k}, Y_{1}^{k}\right), \ldots,\left(X_{n}^{k}, Y_{n}^{k}\right), X_{n+1}^{k}$

## A simple binomial test

- For each data set $k=1, \ldots,\lfloor\kappa\rfloor$, fit models

$$
\widehat{f}_{k}=\mathcal{A}\left(\left(X_{i}^{k}, Y_{i}^{k}\right)_{i \in[n]}\right), \quad \widehat{f}_{k}^{n}=\mathcal{A}\left(\left(X_{i}^{k}, Y_{i}^{k}\right)_{i \in[n-1]}\right)
$$

\& compare predictions:

$$
\Delta_{k}=\left|\widehat{f}_{k}\left(X_{n+1}^{k}\right)-\widehat{f}_{k}^{\backslash n}\left(X_{n+1}^{k}\right)\right|
$$

- Compare against Binom $(\lfloor\kappa\rfloor, \delta)$ at level $\alpha$ :

$$
\widehat{T}=\mathbf{1}\left\{\sum_{k} \mathbf{1}_{\Delta_{k}>\epsilon} \leq \text { the } \alpha \text {-quantile of } \operatorname{Binom}(\lfloor\kappa\rfloor, \delta)\right\}
$$

## Performance of the binomial test

Theorem: validity of the simple binomial test
If $(\mathcal{A}, P, n)$ is not $(\epsilon, \delta)$-stable, then

$$
\mathbb{P}\{\widehat{T}=1\} \leq \alpha
$$

Theorem: power of the simple binomial test If $(\mathcal{A}, P, n)$ is $(\epsilon, \delta)$-stable, \& either $\delta_{\epsilon}^{*}=0$ or $\delta \leq 1-\alpha^{1 /\lfloor\kappa\rfloor}$,

$$
\mathbb{P}\{\widehat{T}=1\}=\left\{\alpha \cdot\left(\frac{1-\delta_{\epsilon}^{*}}{1-\delta}\right)^{\lfloor\kappa\rfloor}\right\} \wedge 1
$$

$$
\delta_{\epsilon}^{*}=\min \{\delta:(\mathcal{A}, P, n) \text { is }(\epsilon, \delta) \text {-stable }\}
$$

## Performance of the binomial test

- The binomial test has validity, but power is low
- Unsurprising $b / c$ it doesn't make efficient use of the datacan we improve power by extracting more info from the data?


## A hardness result

Recall $\kappa=\min \left\{\frac{\left|\mathcal{D}_{\ell}\right|}{n}, \frac{\left|\mathcal{D}_{\ell}\right|+\left|\mathcal{D}_{u}\right|}{n+1}\right\}$

## Theorem: upper bound on power

Let $\widehat{T}$ be any black-box test of stability that is valid at level $\leq \alpha$. If $(\mathcal{A}, P, n)$ is $(\epsilon, \delta)$-stable,

$$
\mathbb{P}\{\widehat{T}=1\} \leq\left\{\alpha \cdot\left(\frac{1-\delta_{\epsilon}^{*}}{1-\delta}\right)^{\kappa}\right\} \wedge 1 .
$$

## A hardness result

Interpretation:

- Every valid black-box test has low power:

$$
\text { if } \kappa=\mathcal{O}(1) \text { and } \delta=o(1) \text { then power } \approx \alpha
$$

- Can't improve on the power of the simple binomial test
- No information can be gained from additional calls to $\mathcal{A}$ or from resampling/bootstrapping/simulating/modeling/etc


## Proof sketch

Suppose $(\mathcal{A}, P, n)$ is $(\epsilon, \delta)$-stable.
Proof idea: construct $\left(\mathcal{A}^{\prime}, P^{\prime}, n\right)$ that is not stable, such that:

- $P \approx P^{\prime}$ so that $\mathrm{d}_{\mathrm{TV}}\left(\right.$ data from $P$, data from $\left.P^{\prime}\right)$ is small
- And, if data $\sim P$, then $\mathcal{A}$ and $\mathcal{A}^{\prime}$ return the same output
- So, $\mathbb{P}_{(\mathcal{A}, P, n)}\{\widehat{T}=1\} \approx \mathbb{P}_{\left(\mathcal{A}^{\prime}, P^{\prime}, n\right)}\{\hat{T}=1\} \leq \alpha$


## Proof sketch

$$
\mathbb{P}\{\widehat{T}=1\} \leq \alpha\left(\frac{1-\delta_{\epsilon}^{*}}{1-\delta}\right)^{\frac{\left|\mathcal{D}_{e}\right|}{n}}
$$

Distribution $P^{\prime}: \operatorname{draw}(X, Y) \sim P$, then return

$$
\begin{cases}(X, Y) & \text { with probability } 1-c \\ \left(X, y_{*}\right) & \text { with probability } c \\ & \text { for a small constant } c>0\end{cases}
$$

## Proof sketch

$\mathbb{P}\{\widehat{T}=1\} \leq \alpha\left(\frac{1-\delta_{\epsilon}^{*}}{1-\delta}\right)^{\frac{\left|\mathcal{D}_{e}\right|}{n}}$

Distribution $P^{\prime}: \operatorname{draw}(X, Y) \sim P$, then return

$$
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$$

Algorithm $\mathcal{A}^{\prime}$ :
Given data $\left(x_{1}, y_{1}\right), \ldots,\left(x_{m}, y_{m}\right) \&$ test point $x_{m+1}$,

- If $m=n$ and $y_{i}=y_{*}$ for any $i$, return a corrupted prediction
- Otherwise, return $\left[\mathcal{A}\left(\left(x_{1}, y_{1}\right), \ldots,\left(x_{m}, y_{m}\right)\right)\right]\left(x_{m+1}\right)$


## Proof sketch

$\mathbb{P}\{\widehat{T}=1\} \leq \alpha\left(\frac{1-\delta_{\epsilon}^{*}}{1-\delta}\right)^{\frac{\left|D_{\ell}\right|}{n}}$

Distribution $P^{\prime}: \operatorname{draw}(X, Y) \sim P$, then return

$$
\left\{\begin{array}{l}
(X, Y) \\
\left(X, y_{*}\right)
\end{array}\right.
$$

with probability $1-c$
with probability $c$,
for a small constant $c>0$
Algorithm $\mathcal{A}^{\prime}$ :
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## Proof sketch

$$
\mathbb{P}\{\widehat{T}=1\} \leq \alpha\left(\frac{1-\delta_{\epsilon}^{*}}{1-\delta}\right)^{\frac{\left|D_{\ell}\right|}{n}} \text { and } \mathbb{P}\{\widehat{T}=1\} \leq \alpha\left(\frac{1-\delta_{\epsilon}^{*}}{1-\delta}\right)^{\frac{\left|\mathcal{D}_{\ell}\right|+\left|D_{u}\right|}{n+1}}
$$

Distribution $P^{\prime}$ : draw $(X, Y) \sim P$, then return

$$
\begin{cases}(X, Y) & \text { with probability } 1-c \\ (X /, \mid y, k)\left(x_{*}, Y\right) & \text { with probability } c\end{cases}
$$

Algorithm $\mathcal{A}^{\prime}$ :
choose s.t. $\left(\mathcal{A}^{\prime}, P^{\prime}, n\right)$
is not $(\epsilon, \delta)$ stable
Given data $\left(x_{1}, y_{1}\right), \ldots,\left(x_{m}, y_{m}\right) \&$ test point $x_{m+1}$,

$$
x_{i}=x_{*}
$$

- If $m=n$ and $y_{i} / \nmid H \mid x \nmid k$ for any $i$, return a corrupted prediction
- Otherwise, return $\left[\mathcal{A}\left(\left(x_{1}, y_{1}\right), \ldots,\left(x_{m}, y_{m}\right)\right)\right]\left(x_{m+1}\right)$


## Part 1: summary \& open questions

Our results:

- The simple binomial test uses the data very inefficiently, but can still be the most powerful distribution-free test of stability
- More sophisticated strategies (simulating/bootstrapping/etc) do not help to determine stability


## Part 1: summary \& open questions

Our results:

- The simple binomial test uses the data very inefficiently, but can still be the most powerful distribution-free test of stability
- More sophisticated strategies (simulating/bootstrapping/etc) do not help to determine stability

Open questions:

- Are there mild assumptions on $\mathcal{A}, P$ that make stability testable?
- Are we using a definition of stability that's too strong?
- Is there a way to convert any algorithm into a stable algorithm, with a pre- or post-processing step?


## Part 2: Stability of bagged algorithms

## Question inspired by Part 1

- Is there a way to convert any algorithm into a stable algorithm?

Empirically, bagging (\& other ensembling procedures) have been observed to improve stability dramatically.

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- Is there a way to convert any algorithm into a stable algorithm?

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## Bagging

- Sample subsets $S_{b} \subseteq[n]$ for $b=1, \ldots, B$
- Fit models $\widehat{f}_{b}=\mathcal{A}\left(\left(X_{i}, Y_{i}\right): i \in S_{b}\right)$
- $\mathcal{A}_{\text {bag }}$ returns aggregated model $\widehat{f}$ :

$$
\widehat{f}(x):=\frac{1}{B} \sum_{b} \widehat{f}_{b}(x)
$$

## Background on bagging

The most common options:

- Classical bagging $=$ subsets $S_{b}$ of size $m$, sampled $w /$ replacement

$$
p=\mathbb{P}\left\{i \in S_{b}\right\}=1-(1-1 / n)^{m}
$$

- Subbagging $=$ subsets $S_{b}$ of size $m<n$, sampled $w /$ o replacement

$$
p=\mathbb{P}\left\{i \in S_{b}\right\}=m / n
$$

## Background on bagging

Bagging appears in:

- Random forests [Breiman 2001]
- Variable selection in regression [Meinshausen \& Bühlmann 2010]
- Classification in the presence of class imbalance [Li 2007]
- Robust Bayesian inference (BayesBag) [Huggins \& Miller 2023]
- \& many more


## Background on bagging

Many results on theoretical properties-
Bagging induces smoothness, reduces variance, creates robustness
[Bühlmann\&Yu 2002, Grandvalet 2004, Friedman\&Hall 2000, Elisseeff et al 2005, ...]

Some results show stability of bagging in limited regimes ( $m \ll n$ ) [Poggio et al 2002, Chen et al 2022]

## Bagging helps stability



## Re-defining stability

## Definition from Part 1

$\mathcal{A}$ is $(\epsilon, \delta)$-stable if

$$
\mathbb{P}_{P}\left\{\left|\widehat{f}(x)-\widehat{f}^{i}(x)\right|>\epsilon\right\} \leq \delta
$$

when trained on $\mathcal{D}=\left(X_{1}, Y_{1}\right), \ldots,\left(X_{n}, Y_{n}\right) \stackrel{\text { iid }}{\sim} P$, and tested on $x \sim P_{X}$

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## Updated definition (strictly stronger)

$\mathcal{A}$ is $(\epsilon, \delta)$-stable if

$$
\frac{1}{n} \sum_{i=1}^{n} \mathbb{1}\left\{\left|\widehat{f}(x)-\widehat{f}^{\backslash i}(x)\right|>\epsilon\right\} \leq \delta
$$

when trained on any $\mathcal{D}=\left(X_{1}, Y_{1}\right), \ldots,\left(X_{n}, Y_{n}\right)$, and tested on any $x$

## Main result: stability guarantee

$$
\text { Recall } p=\mathbb{P}\left\{i \in S_{b}\right\}= \begin{cases}m / n & \text { for subbagging } \\ 1-(1-1 / n)^{m} & \text { for classical bagging }\end{cases}
$$

## Theorem

Let $\mathcal{A}$ be any base algorithm that returns predictions in $[0,1]$.
For any $n, m$, as $B \rightarrow \infty, \mathcal{A}_{\text {bag }}$ satisfies $(\epsilon, \delta)$-stability for every

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\delta \epsilon^{2} \geq \frac{1}{4(n-1)} \cdot \frac{p}{1-p}
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- Framework \& results allow for a randomized $\mathcal{A}$
- Results extend to finite $B$ (use Hoeffding's inequality)
- Can also extend to models with unbounded output, via either clipping predictions, or letting $\epsilon$ adapt to the range of $\widehat{f}$


## Main result: stability guarantee

Regimes for subbagging:

- Proportional sampling: $m=\mathcal{O}(n)$

Stability is guaranteed for $\delta \epsilon^{2} \gtrsim n^{-1}$

- Massive subsampling: $m=\mathcal{O}\left(n^{\beta}\right)$ for $0<\beta<1$

Stability is guaranteed for $\delta \epsilon^{2} \gtrsim n^{-(2-\beta)}$
[See also existing stability guarantees by Chen, Syrgkanis, Austern 2022]

- Minimal subsampling: $m=n-\mathcal{O}\left(n^{\beta}\right)$ for $0<\beta<1$ Stability is guaranteed for $\delta \epsilon^{2} \gtrsim n^{-\beta}$


## Proof sketch

Suppose $S \subset[n]$ contains $\delta n$ "bad" data points:

$$
\left|\widehat{f}(x)-\widehat{f}^{i}(x)\right| \geq \epsilon
$$

where $\widehat{f}=\mathcal{A}_{\text {bag }}(\mathcal{D})$ averages over all bags $S_{b}$, while $\widehat{f}^{i}=\mathcal{A}_{\text {bag }}\left(\mathcal{D}_{-i}\right)$ averages over all bags $S_{b} \not \nexists i$.

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Proof idea: a double counting argument for $L=\sum_{i \in S}|\widehat{f}(x)-\widehat{f} \backslash i(x)|$

- Summing over $i$, we see $L \geq \epsilon \cdot|S|=\delta \epsilon n$
- We can also rewrite $L$ by summing over bags $b$, because

$$
\widehat{f}^{\backslash}(x)=\mathbb{E}\left[\widehat{f}_{b}(x) \mid i \notin S_{b}\right]=\frac{1}{1-p} \mathbb{E}\left[\widehat{f}_{b}(x) \mathbb{1}_{i \in S_{b}}\right]
$$

where expectation is taken over a randomly drawn bag $S_{b}$.

## Empirical results

Neural networks


## Empirical results

Regression trees


## Empirical results

Logistic regression + ridge penalty with $\lambda=0.001$


## Is the guarantee tight?

## Theorem: a matching bound for subbagging

There exists a base algorithm $\mathcal{A}$ that returns predictions in $[0,1]$, such that as $B \rightarrow \infty, \mathcal{A}_{\text {bag }}$ is not $(\epsilon, \delta)$-stable for any

$$
\delta \epsilon^{2}<\frac{1}{c(n-1)} \cdot \frac{p}{1-p}
$$

for a constant $c$, as long as $1 / n \ll \delta \leq 1 / 2$ and $\min \{p, 1-p\} \gg 1 / n$.

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Illustration for $n=500, m=250$ :


## Is the guarantee tight?

Proof sketch: a "voting" algorithm

- Let $X_{i}=1$ for $\delta n$ many $i \in[n]$, otherwise $X_{i}=0$
- Want to construct $\mathcal{A}$ so that $\left|\widehat{f}(x)-\widehat{f}{ }^{i}(x)\right| \geq \epsilon$ for all $i$ with $X_{i}=1$


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- Want to construct $\mathcal{A}$ so that $\left|\widehat{f}(x)-\widehat{f}{ }^{i}(x)\right| \geq \epsilon$ for all $i$ with $X_{i}=1$
- Let $\widehat{f}_{b}(x)=\mathbb{1}_{\sum_{i \in b} x_{i} \geq t}$ for some $t \approx p \delta$
- If $X_{i}=1$, then $i \in S_{b} \Rightarrow \widehat{f}_{b}(x)$ is a bit more likely to be 1
- If $X_{i}=0$, then $i \in S_{b} \Rightarrow \widehat{f}_{b}(x)$ is a bit more likely to be 0
- Exact probabilities calculated via the HyperGeometric distrib


## Stability definitions

Compare to a more strict definition of stability:

## Worst-case stability

$\mathcal{A}$ is $\epsilon$-worst-case-stable if

$$
\max _{i}|\widehat{f}(x)-\widehat{f} \backslash i(x)| \leq \epsilon \quad \leftarrow \text { rather than } \sum_{i} \mathbb{1}_{\left|\widehat{f}(x)-\widehat{f}{ }^{i}(x)\right|>\epsilon} \leq \delta n
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Results (with $B \rightarrow \infty$ ):

- For any $\mathcal{A}, \mathcal{A}_{\text {bag }}$ is $p$-worst-case-stable
- For any $\epsilon<p$, there exists an $\mathcal{A}$ s.t. $\mathcal{A}_{\text {bag }}$ is not $\epsilon$-worst-case-stable


## Part 2: summary \& open questions

Our results:

- Classical bagging \& subbagging can be applied to any algorithm $\mathcal{A}$ to achieve an assumption-free stability guarantee
- Downstream, this verifies generalization, predictive inference, etc properties for bagged algorithms


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- Classical bagging \& subbagging can be applied to any algorithm $\mathcal{A}$ to achieve an assumption-free stability guarantee
- Downstream, this verifies generalization, predictive inference, etc properties for bagged algorithms

Open questions:

- How does bagging perform relative to other definitions of stability?
- Guarantees for aggregation procedures aside from averaging?
- Guarantees for structured prediction problems $(\mathcal{Y} \nsubseteq \mathbb{R})$ ?


[^0]:    ${ }^{1}$ Kim \& B., Black-box tests for algorithmic stability, arXiv: 2111.15546
    ${ }^{2}$ Soloff, B., \& Willett, Bagging provides assumption-free stability, arxiv:2301.12600

