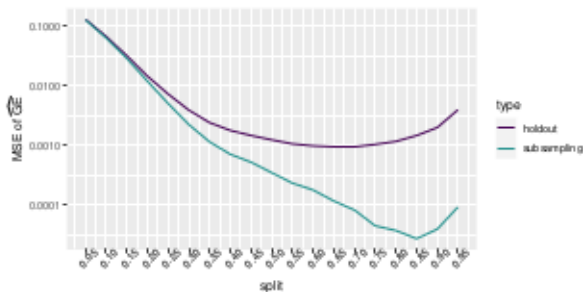


BIAS-VARIANCE ANALYSIS FOR SUBSAMPLING



- MSE of \widehat{GE} strictly better for SS
- Smaller var of SS enables to use larger s for optimal choice
- The optimal split rate now is a higher $s \approx 0.8$.
- Beyond $s = 0.8$: MSE goes up because var doesn't go down as much as we want due to increasing overlap in trainsets (see later)

DEDICATED TESTSET SCENARIO - ANALYSIS

- Goal: estimate $GE(\hat{f}) = E[L(y, \hat{f}(\mathbf{x}))]$ via

$$\widehat{GE}(\hat{f}) = \frac{1}{m} \sum_{(\mathbf{x}, y) \in \mathcal{D}_{\text{test}}} L(y, \hat{f}(\mathbf{x}))$$

Here, only (\mathbf{x}, y) are random, they are i.i.d. fresh test samples

- This is: average over i.i.d $L(y, \hat{f}(\mathbf{x}))$, so directly know E and var.
And can use CLT to approx distrib of $\widehat{GE}(\hat{f})$ with Gaussian.
- $E[\widehat{GE}(\hat{f})] = E[L(y, \hat{f}(\mathbf{x}))] = GE(\hat{f})$
- $V[\widehat{GE}(\hat{f})] = \frac{1}{m} V[L(y, \hat{f}(\mathbf{x}))]$
- So $\widehat{GE}(\hat{f})$ is unbiased estimator of $GE(\hat{f})$, var decreases linearly in testset size, have an approx of full distrib (can do NHST, CIs, etc.)
- NB: Gaussian may work less well for e.g. 0-1 loss, with E close to 0, can use binomial or other special approaches for other losses



PESSIMISTIC BIAS IN RESAMPLING

- Estim $GE(\mathcal{I}, n)$ (surrogate for $GE(\hat{f})$) when \hat{f} is fit on full \mathcal{D} , with $|\mathcal{D}| = n$) via resampling based estim $\widehat{GE}(\mathcal{I}, n_{\text{train}})$

$$\widehat{GE}(\mathcal{I}, \mathcal{J}, \rho, \lambda) = \text{agr} \left(\rho \left(\mathbf{y}_{\mathcal{J}_{\text{test},1}}, \mathbf{F}_{\mathcal{J}_{\text{test},1}, \mathcal{I}(\mathcal{D}_{\text{train},1}, \lambda)} \right), \right. \\ \vdots \\ \left. \rho \left(\mathbf{y}_{\mathcal{J}_{\text{test},B}}, \mathbf{F}_{\mathcal{J}_{\text{test},B}, \mathcal{I}(\mathcal{D}_{\text{train},B}, \lambda)} \right) \right),$$

- Let's assume agr is avg and ρ is loss-based, so ρ_L
- The ρ are simple holdout estims. So:

$$\mathbf{E}[\widehat{GE}(\mathcal{I}, \mathcal{J}, \rho, \lambda)] \approx \mathbf{E}[\rho(\mathbf{y}_{\mathcal{J}_{\text{test}}}, \mathbf{F}_{\mathcal{J}_{\text{test}}, \mathcal{I}(\mathcal{D}_{\text{train}}, \lambda)})]$$

- NB1: In above, as always for $GE(\mathcal{I})$, both $\mathcal{D}_{\text{train}}$ and $\mathcal{D}_{\text{test}}$ (and so $\mathbf{x} \in \mathcal{D}_{\text{test}}$) are random vars, and we take E over them
- NB2: Need \approx as maybe not all train/test sets in resampling of exactly same size



$$\mathbf{E}[\widehat{GE}(\mathcal{I}, \mathcal{J}, \rho, \lambda)] \approx \mathbf{E}[\rho(\mathbf{y}_{\mathcal{J}_{\text{test}}}, \mathbf{F}_{\mathcal{J}_{\text{test}}; \mathcal{I}(\mathcal{D}_{\text{train}}; \lambda)})] =$$

$$\mathbf{E} \left[\frac{1}{m} \sum_{\substack{(\mathbf{x}, y) \in \mathcal{D}_{\text{test}} \\ (\mathbf{x}, y) \in \mathcal{D}_{\text{test}}}} L(y, \mathcal{I}(\mathcal{D}_{\text{train}})(\mathbf{x})) \right] \equiv GE(\mathcal{I}, n_{\text{train}})$$

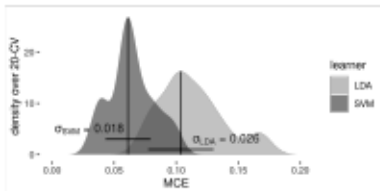


- So when we use $\widehat{GE}(\mathcal{I}, \mathcal{J}, \rho, \lambda)$ to estimate $GE(\mathcal{I}, n)$, our expected value is nearly correct, it's $GE(\mathcal{I}, n_{\text{train}})$
- But fitting \mathcal{I} on less data (n_{train} vs full n) usually results in model with worse perf, hence estimator is pessimistically biased
- Bias the stronger, the smaller our training splits in resampling.

NO INDEPENDENCE OF CV RESULTS

- Similar analysis as before holds for CV
- Might be tempted to report distribution or SD of individual CV split perf values, e.g. to test if perf of 2 learners is significantly different
- But k CV splits are not independent

A t-test on the difference of the mean GE estimators yields a highly significant p-value of $\approx 7.9 \cdot 10^{-5}$ on the 95% level.

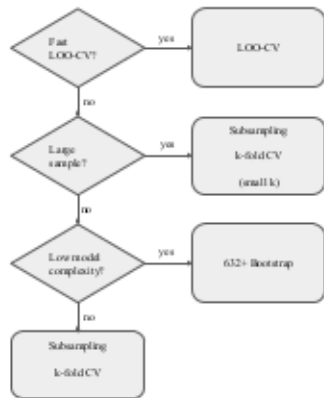


LDA vs SVM on a pass classification problem, performance estimation via 20-CV w.r.t. MCE.

NO INDEPENDENCE OF CV RESULTS

- $\mathbb{V}[\widehat{GE}]$ of CV is a difficult combination of
 - average variance as we estim on finite trainsets
 - covar from test errors, as models result from overlapping trainsets
 - covar due to the dependence of trainsets and test obs appear in trainsets
- Naively using the empirical var of k individual \widehat{GE} s (as on slide before) yields biased estimator of $\mathbb{V}[\widehat{GE}]$. Usually this underestimates the true var!
- Worse: there is no unbiased estimator of $\mathbb{V}[\widehat{GE}]$ [Bengio, 2004]
- Take into account when comparing learners by NHST
- Somewhat difficult topic, we leave it with the warning here

SHORT GUIDELINE



- 5-CV or 10-CV have become standard.
- Do not use hold-out, CV with few folds, or SS with small split rate for small n . Can bias estim and have large var.
- For small n , e.g. $n < 200$, use LOO or, probably better, repeated CV.
- For some models, fast tricks for LOO exist
- With $n = 100,000$, can have "hidden" small-sample size, e.g. one class very small
- SS usually better than bootstrapping. Repeated obs can cause problems in training, especially in nested setups where the "training" set is split up again.