Why would φ_B be any better than φ ?

Illustration on the regression case:

Suppose (X,Y) drawn from distribution $P_{X,Y}$. φ predictor trained on $\mathcal T$ or any bootstrap sample of $\mathcal T$ $\hat{P}_{\mathcal T} \text{ empirical distribution of } \mathcal T$ $P_{\mathcal T} \text{ true distribution of } \mathcal T$ To simplify notation: $\mathbb E_{P_{X,Y}} = \mathbb E_{X,Y}, \ \mathbb E_{P_{\mathcal T}} = \mathbb E_{\mathcal T} \text{ and } \mathbb E_{\hat{P}_{\mathcal T}} = \mathbb E_{\hat{\mathcal T}}.$ $\varphi_B(\cdot) = \mathbb E_{\hat{\mathcal T}} \left(\varphi(\cdot) \right) \text{ Bagging predictor}$ $\varphi_A(\cdot) = \mathbb E_{\mathcal T} \left(\varphi(\cdot) \right) \text{ aggregated predictor}$

Average prediction error of
$$\varphi_A$$
: $e_A = \mathbb{E}_{X,Y}\left(\left[Y - \varphi_A\left(X\right)\right]^2\right)$.

Average prediction error of φ : $e = \mathbb{E}_{\mathcal{T}}\left(\mathbb{E}_{X,Y}\left([Y - \varphi(X)]^2\right)\right)$. Average prediction error of φ_A : $e_A = \mathbb{E}_{X,Y}\left([Y - \varphi_A(X)]^2\right)$.

Average prediction error of
$$\varphi_{A}$$
. $e_{A} = \mathbb{E}_{X,Y}\left(\left[T - \varphi_{A}\left(X\right)\right]\right)$.
$$e = \mathbb{E}_{X,Y}\left(Y^{2}\right) - 2\mathbb{E}_{X,Y}\left(\mathbb{E}_{\mathcal{T}}\left(Y\varphi\left(X\right)\right)\right) + \mathbb{E}_{X,Y}\left(\mathbb{E}_{\mathcal{T}}\left(\left[\varphi(X)\right]^{2}\right)\right)$$

Average prediction error of φ : $e = \mathbb{E}_{\mathcal{T}}\left(\mathbb{E}_{X,Y}\left([Y-\varphi(X)]^2\right)\right)$. Average prediction error of φ_A : $e_A = \mathbb{E}_{X,Y}\left([Y-\varphi_A(X)]^2\right)$. $e = \mathbb{E}_{X,Y}\left(Y^2\right) - 2\mathbb{E}_{X,Y}\left(\mathbb{E}_{\mathcal{T}}\left(Y\varphi(X)\right)\right) + \mathbb{E}_{X,Y}\left(\mathbb{E}_{\mathcal{T}}\left([\varphi(X)]^2\right)\right)$

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$$e = \mathbb{E}_{X,Y} \left(Y^2 - 2\mathbb{E}_{X,Y} \left(Y(\varphi_A(X)) + \mathbb{E}_{X,Y} \left(\mathbb{E}_{\mathcal{T}} \left([\varphi(X)]^2 \right) \right) \right)$$

$$e = \mathbb{E}_{X,Y}\left(Y^2\right) - 2\mathbb{E}_{X,Y}\left(Y\varphi_A(X)\right) + \mathbb{E}_{X,Y}\left(\mathbb{E}_{\mathcal{T}}\left(\left[\varphi(X)\right]^2\right)\right)$$
 But $\mathbb{E}_{X,Y}\left(\mathbb{E}_{\mathcal{T}}\left(\left[\varphi(X)\right]^2\right)\right) \ge \mathbb{E}_{X,Y}\left(\left[\varphi_A(X)\right]^2\right)$

So $e > e_A$.

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But
$$\mathbb{E}_{X,Y}\left(\mathbb{E}_{\mathcal{T}}\left(\left[\varphi(X)\right]^{2}\right)\right) \geq \mathbb{E}_{X,Y}\left(\left[\varphi_{A}(X)\right]^{2}\right)$$

So $e \geq e_{A}$.
Moreover:
 $e - e_{A} = \mathbb{E}_{X,Y}\left(\mathbb{E}_{\mathcal{T}}\left(\left[\varphi(X)\right]^{2}\right) - \left[\mathbb{E}_{\mathcal{T}}\left(\varphi(X)\right]^{2}\right)$

$$\begin{aligned} & \text{Moreover:} \\ & e - e_A = \mathbb{E}_{X,Y} \left(\mathbb{E}_{\mathcal{T}} \left(\left[\varphi(X) \right]^2 \right) - \left[\mathbb{E}_{\mathcal{T}} \left(\varphi(X) \right) \right]^2 \right) \\ & e - e_A = \mathbb{E}_{X,Y} \left(\mathbb{E}_{\mathcal{T}} \left(\left[\varphi(X) \right]^2 \right) - \left[\varphi_A(X) \right]^2 \right) \end{aligned}$$

Average prediction error of φ : $e = \mathbb{E}_{\mathcal{T}}\left(\mathbb{E}_{X,Y}\left([Y-\varphi(X)]^2\right)\right)$. Average prediction error of φ_A : $e_A = \mathbb{E}_{X,Y}\left([Y-\varphi_A(X)]^2\right)$. $e = \mathbb{E}_{X,Y}\left(Y^2\right) - 2\mathbb{E}_{X,Y}\left(Y\varphi_A(X)\right) + \mathbb{E}_{X,Y}\left(\mathbb{E}_{\mathcal{T}}\left([\varphi(X)]^2\right)\right)$ But $\mathbb{E}_{X,Y}\left(\mathbb{E}_{\mathcal{T}}\left([\varphi(X)]^2\right)\right) \geq \mathbb{E}_{X,Y}\left([\varphi_A(X)]^2\right)$ So $e \geq e_A$. Moreover: $e - e_A = \mathbb{E}_{X,Y}\left(\mathbb{E}_{\mathcal{T}}\left([\varphi(X)]^2\right) - [\mathbb{E}_{\mathcal{T}}\left(\varphi(X)\right)]^2\right)$

 $e - e_A = \mathbb{E}_{X,Y} \left(\mathbb{E}_{\mathcal{T}} \left([\varphi(X)]^2 \right) - [\varphi_A(X)]^2 \right)$

Interpretation: if $\varphi_{\mathcal{T}}$ differs a lot from $\varphi_{\mathcal{T}'}$, then $e-e_A$ is large. \Rightarrow The highest the variance of φ across training sets \mathcal{T} , the more improvement φ_A produces.

Ok, so φ_A always improves on φ , especially when φ is highly variable w.r.t. changes in \mathcal{T} .

Ok, so φ_A always improves on φ , especially when φ is highly variable w.r.t. changes in $\mathcal T$.

 $\begin{array}{c} \text{But } \varphi_A \text{ is not } \varphi_B. \text{ Recall:} \\ \varphi_A(\cdot) = \mathbb{E}_{\mathcal{T}}\left(\varphi(\cdot)\right) \text{ aggregated predictor (over all N-size training sets)} \\ \varphi_B(\cdot) = \mathbb{E}_{\hat{\mathcal{T}}}\left(\varphi(\cdot)\right) \text{ Bagging predictor (over bootstrap samples)} \\ \varphi_B \text{ approximates } \varphi_A \text{ and thus } e_B \geq e_A \end{array}$

Ok, so φ_A always improves on φ , especially when φ is highly variable w.r.t. changes in $\mathcal T$.

But φ_A is not φ_B . Recall:

$$\begin{split} \varphi_A(\cdot) &= \mathbb{E}_{\mathcal{T}}\left(\varphi(\cdot)\right) \text{ aggregated predictor (over all N-size training sets)} \\ \varphi_B(\cdot) &= \mathbb{E}_{\hat{\mathcal{T}}}\left(\varphi(\cdot)\right) \text{ Bagging predictor (over bootstrap samples)} \\ \varphi_B \text{ approximates } \varphi_A \text{ and thus } e_B \geq e_A \end{split}$$

- lacktriangle If arphi highly variable w.r.t. \mathcal{T} , $arphi_B$ improves on arphi through aggregation.
- ▶ But if φ is rather stable w.r.t. \mathcal{T} , $e_A \approx e$ and since φ_B approximates φ_A , e_B might be greater than e.

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Actually, no, it does not always work.

Bagging should be used to transform highly variable predictors φ into a more accurate averaged commitee φ_B .

Examples of φ that Bagging improve:

- \rightarrow Trees, Neural Networks.
- Examples of φ that Bagging does not improve much (or degrades):
- → Support Vector Machines, Gaussian Processes.

And in the classification case?

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Majority vote:
$$\varphi_B(x) = \arg\max_j \sum_{b=1}^B I(\varphi^b(x) = j)$$

More drastic conclusions:

- ullet arphi unstable w.r.t. ${\mathcal T}$ and reasonable performance $\Rightarrow arphi_B$ near optimal.
- φ stable w.r.t. $\mathcal{T}\Rightarrow \varphi_B$ worse than φ .
- φ poor performance $\Rightarrow \varphi_B$ worse than φ .