Why would  $\varphi_B$  be any better than  $\varphi$ ?

#### Illustration on the regression case:

Suppose (X,Y) drawn from distribution  $P_{X,Y}$ .  $\varphi$  predictor trained on  $\mathcal T$  or any bootstrap sample of  $\mathcal T$   $\hat P_{\mathcal T}$  empirical distribution of  $\mathcal T$   $P_{\mathcal T}$  true distribution of  $\mathcal T$  To simplify notation:  $\mathbb E_{P_{X,Y}} = \mathbb E_{X,Y}$ ,  $\mathbb E_{P_{\mathcal T}} = \mathbb E_{\mathcal T}$  and  $\mathbb E_{\hat P_{\mathcal T}} = \mathbb E_{\hat {\mathcal T}}$ .  $\varphi_B(\cdot) = \mathbb E_{\hat {\mathcal T}}(\varphi(\cdot))$  Bagging predictor  $\varphi_A(\cdot) = \mathbb E_{\mathcal T}(\varphi(\cdot))$  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  $\varphi$ :  $e = \mathbb{E}_{\mathcal{T}}\left(\mathbb{E}_{X,Y}\left([Y - \varphi(X)]^2\right)\right)$ . Average prediction error of  $\varphi_A$ :  $e_A = \mathbb{E}_{X,Y}\left([Y - \varphi_A(X)]^2\right)$ .

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

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

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

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

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

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

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

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

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

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

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

But 
$$\mathbb{E}_{X,Y}\left(\mathbb{E}_{\mathcal{T}}\left(\left[\varphi(X)\right]^{2}\right)\right) \geq \mathbb{E}_{X,Y}\left(\left[\varphi_{A}(X)\right]^{2}\right)$$
  
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  $\varphi$ :  $e = \mathbb{E}_{\mathcal{T}}\left(\mathbb{E}_{X,Y}\left([Y-\varphi(X)]^2\right)\right)$ . Average prediction error of  $\varphi_A$ :  $e_A = \mathbb{E}_{X,Y}\left([Y-\varphi_A(X)]^2\right)$ .  $e = \mathbb{E}_{X,Y}\left(Y^2\right) - 2\mathbb{E}_{X,Y}\left(Y\varphi_A(X)\right) + \mathbb{E}_{X,Y}\left(\mathbb{E}_{\mathcal{T}}\left([\varphi(X)]^2\right)\right)$  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  $\varphi$  across training sets  $\mathcal{T}$ , the more improvement  $\varphi_A$  produces.

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

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

But  $\varphi_A$  is not  $\varphi_B$ . 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  $\varphi$  is rather stable w.r.t.  $\mathcal{T}$ ,  $e_A \approx e$  and since  $\varphi_B$  approximates  $\varphi_A$ ,  $e_B$  might be greater than e.

So it does not always work?

So it does not always work?

Actually, no, it does not always work.

Bagging should be used to transform highly variable predictors  $\varphi$  into a more accurate averaged commitee  $\varphi_B$ .

Examples of  $\varphi$  that Bagging improve:

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

And in the classification case?

And in the classification case?

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.
- $\varphi$  stable w.r.t.  $\mathcal{T}\Rightarrow \varphi_B$  worse than  $\varphi$ .
- $\varphi$  poor performance  $\Rightarrow \varphi_B$  worse than  $\varphi$ .