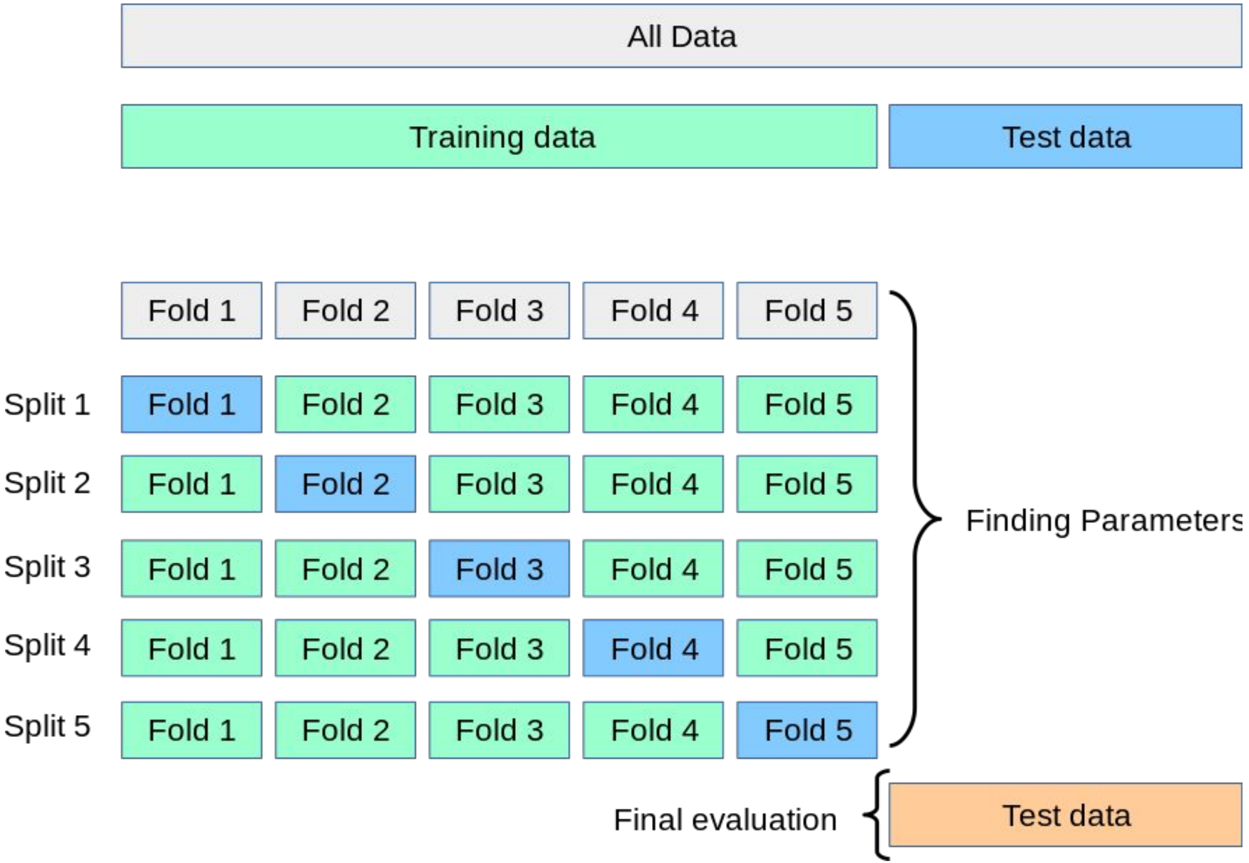
Lecture 8: Bias-Variance tradeoff; More Ensembling

Outline

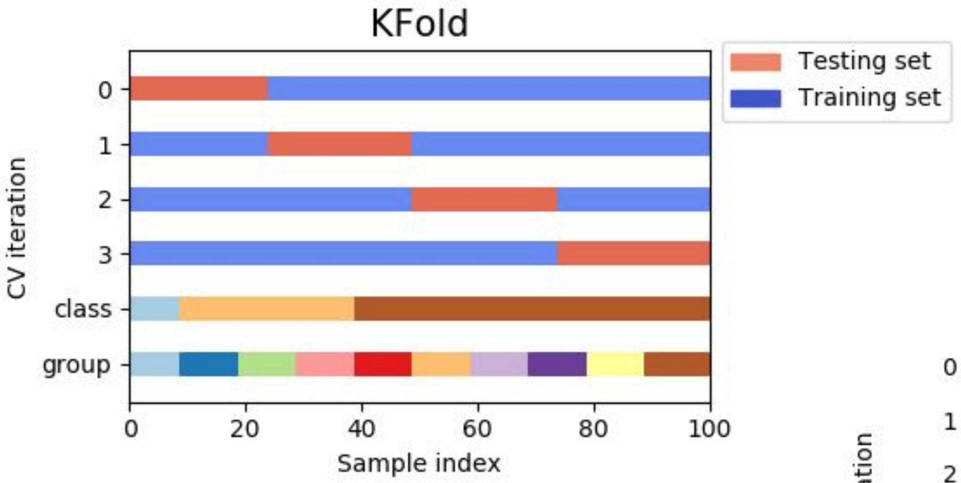
1. Validation Strategies
2. Blending
3. Stacking
4. Bias-Variance Tradeoff

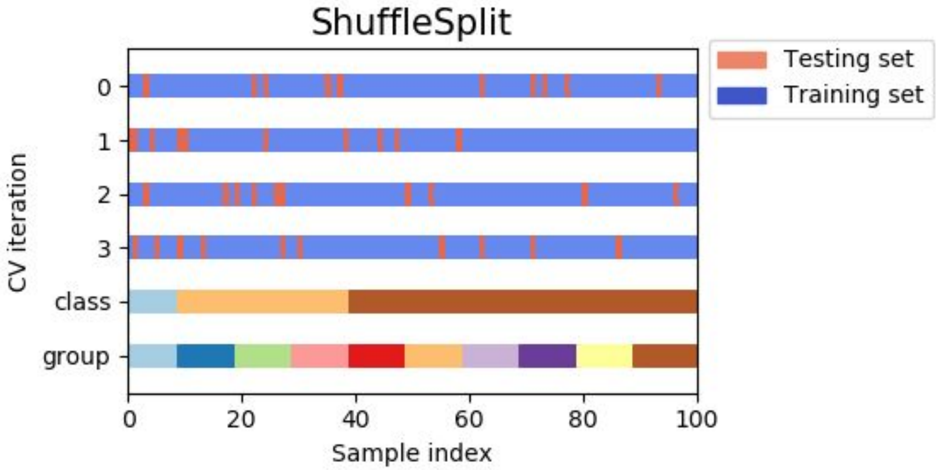
Validation Strategies

Validation strategies



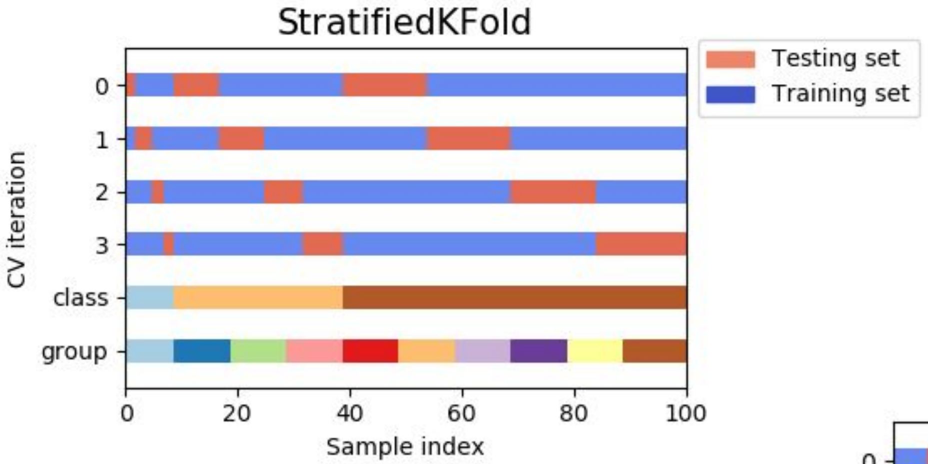
Validation strategies

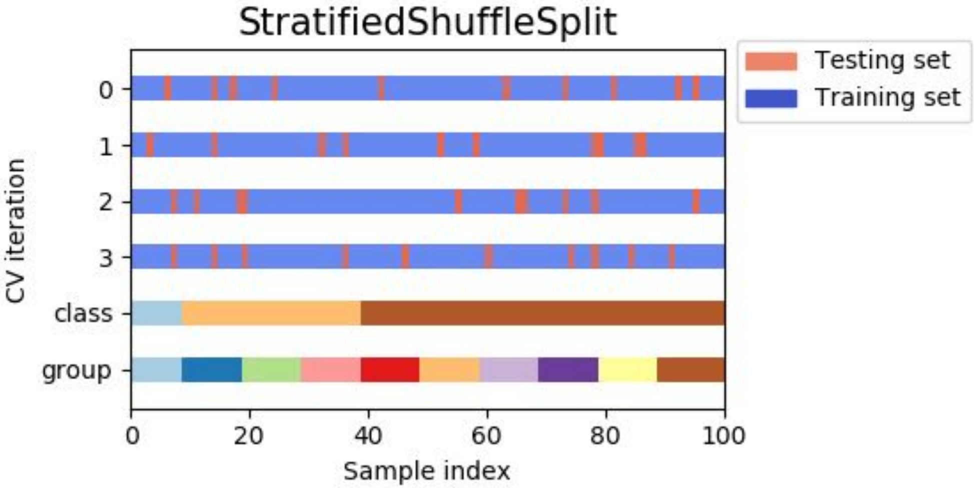




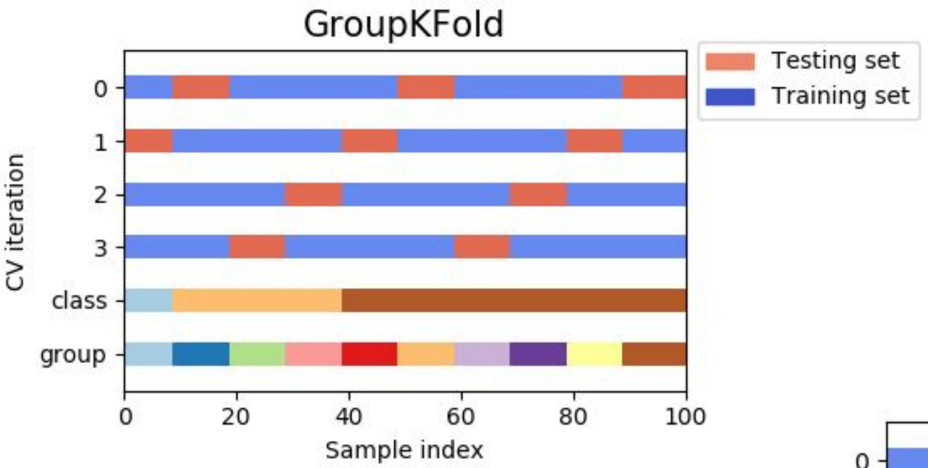
Special case: Leave One Out (LOO) - good for tiny datasets

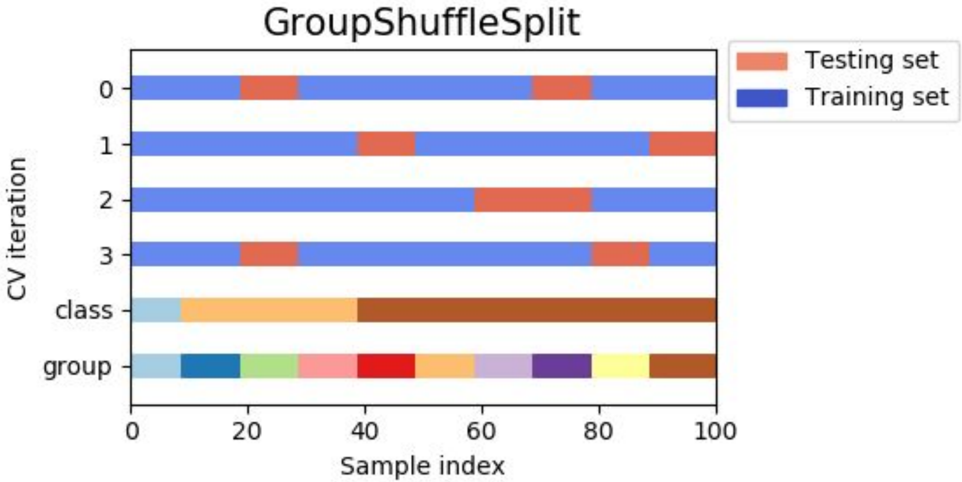
Validation strategies



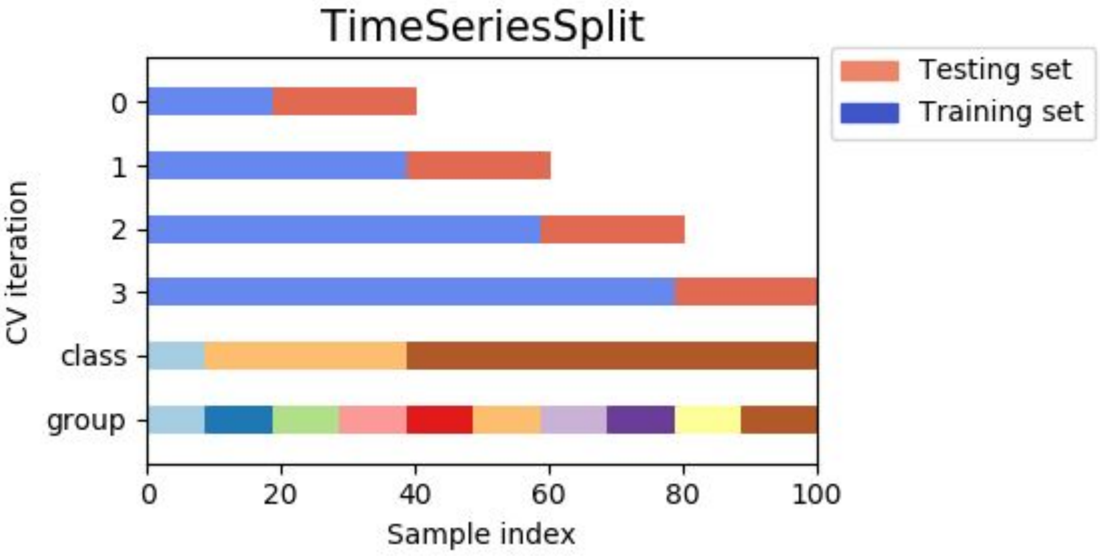


Validation strategies





Special case: time series

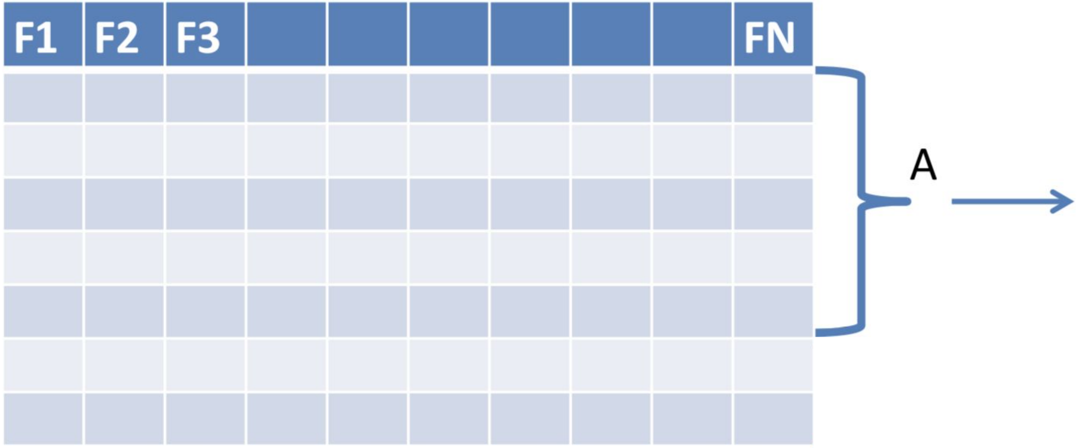


Never use `train_test_split` in this case!

Stacking and blending

Blending

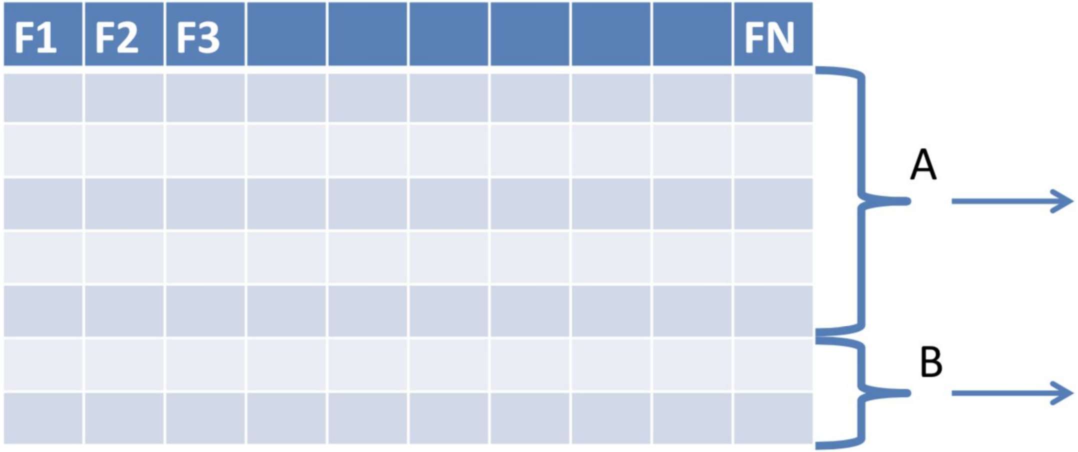
How to build an ensemble from *different* models?



Tune M basic algorithms

Blending

How to build an ensemble from *different* models?

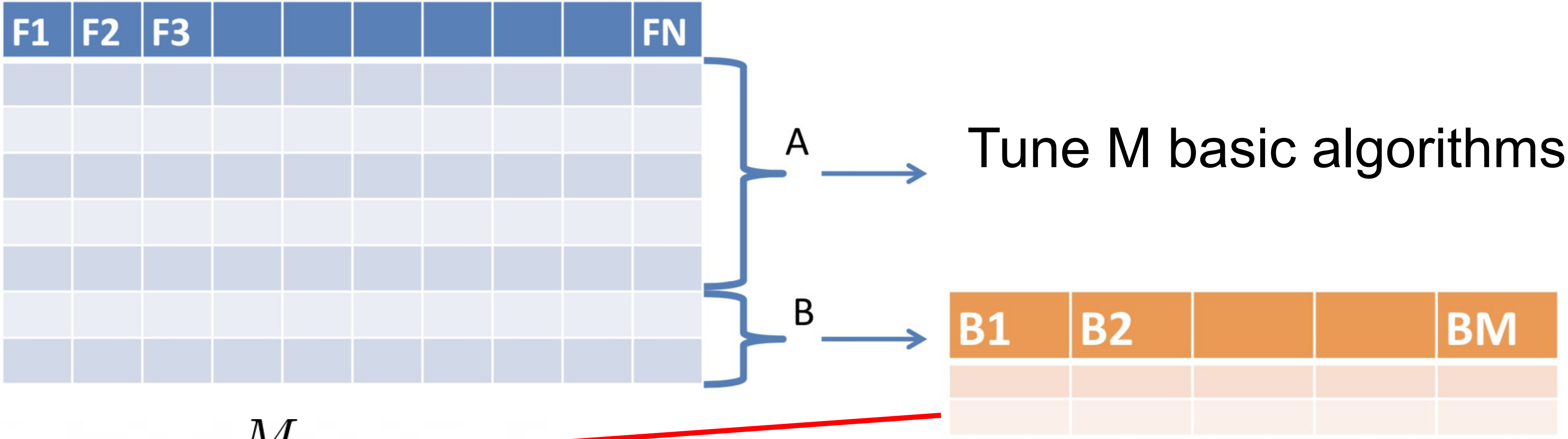


Tune M basic algorithms

Tune new model on the outputs of the basic algorithms

Blending

How to build an ensemble from *different* models?



$$\hat{f}(x) = \sum_{i=1}^{M} \rho_i f_i(x)$$

$$\sum_{i=1}^{M} \rho_i = 1, \quad \rho_i \in [0; 1] \;\; \forall i$$

Blending

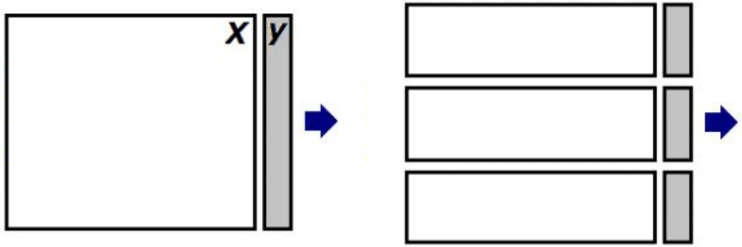
Just combine several *strong/complex* models.

$$\hat{f}(x) = \sum_{i=1}^{M} \rho_i f_i(x), \qquad \sum_{i=1}^{M} \rho_i = 1, \quad \rho_i \in [0; 1] \ \forall i$$

- Pros:
  - Simple and intuitive ensembling method.
  - Average several blendings to achieve better results.
- Cons:
  - Linear composition is not always enough.
  - Need to split the data. How to fix it?

Stacking

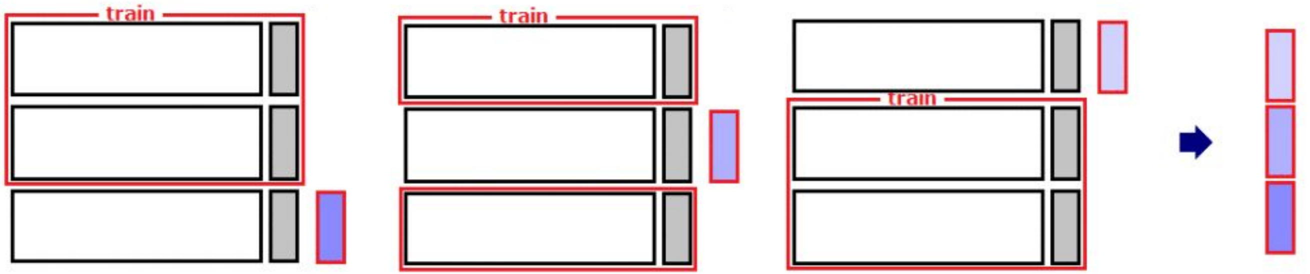
1. Split data into folds

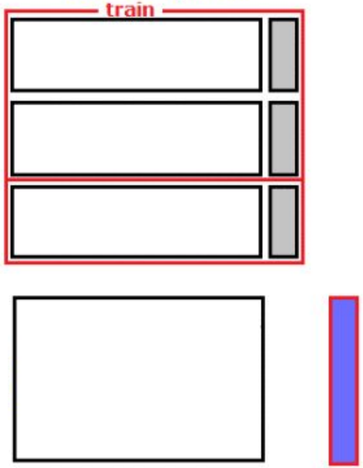


3. Tune the new model on the “meta”-features

Fit using folds to get meta-features on train

Fit using all data meta-features on test





2. Tune models on different groups of folds, predict on left out

Picture source: https://dyakonov.org/2017/03/10/стекинг-stacking-и-блендинг-blending/

Stacking

- Train base algorithm(s) on different groups of folds leaving one fold out.
- Predict the meta-features on the left-out fold and test data.
- Train the meta-algorithm on the meta-features representation of the train data.
- Use it on the meta-features representation of the test data.

Stacking

- Besides $f_i(x)$, i=1,..,M; $\hat{f}(x)$ may also depend on:
  - original features
  - Internal representations in $f_i(x)$ (e.g. class scores)

Stacking

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    - original features
    - Internal representations in $f_i(x)$ (e.g. class scores)

Stacking

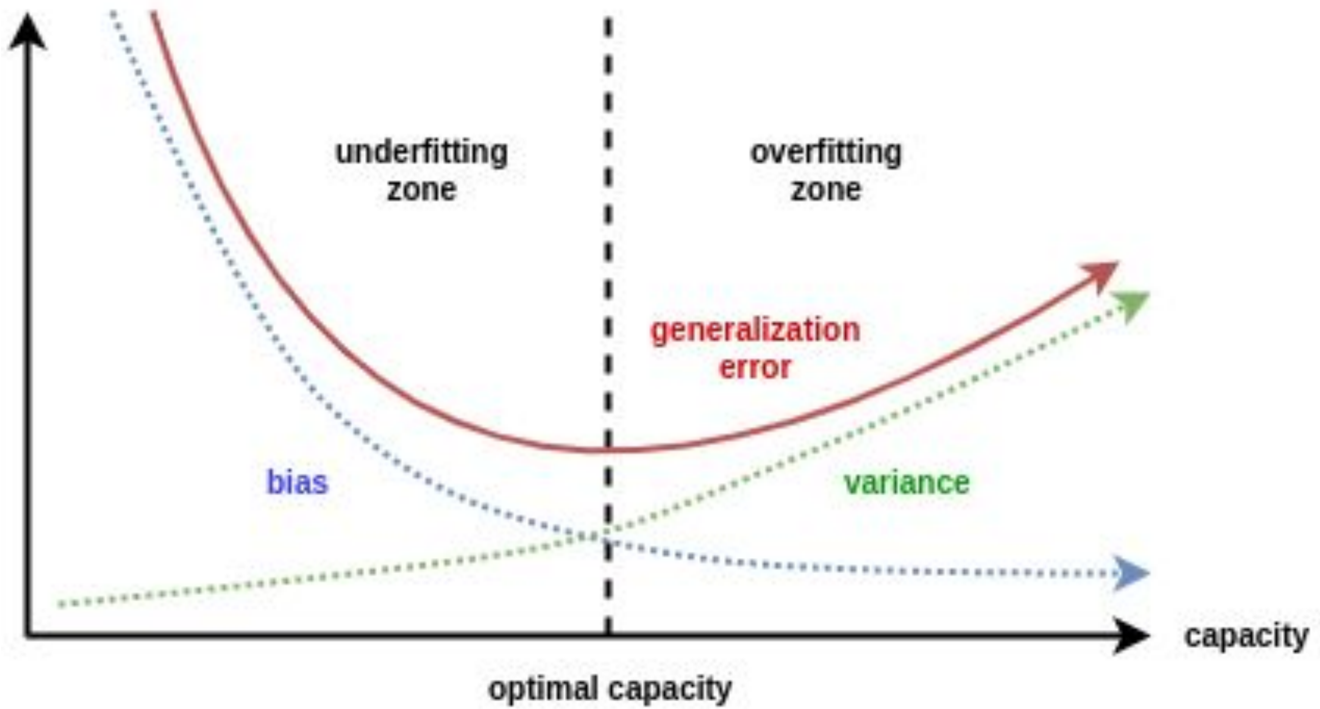
- Pros:
  - Powerful ensembling method, if you know how to use it
  - Quite popular in ML-competitions
  - One might perform stacking on the meta-features dataset as well
- Cons:
  - Meta-features on each fold are actually predicted by different models
    - However, regularization usually helps
  - Hard to explain your model behaviour

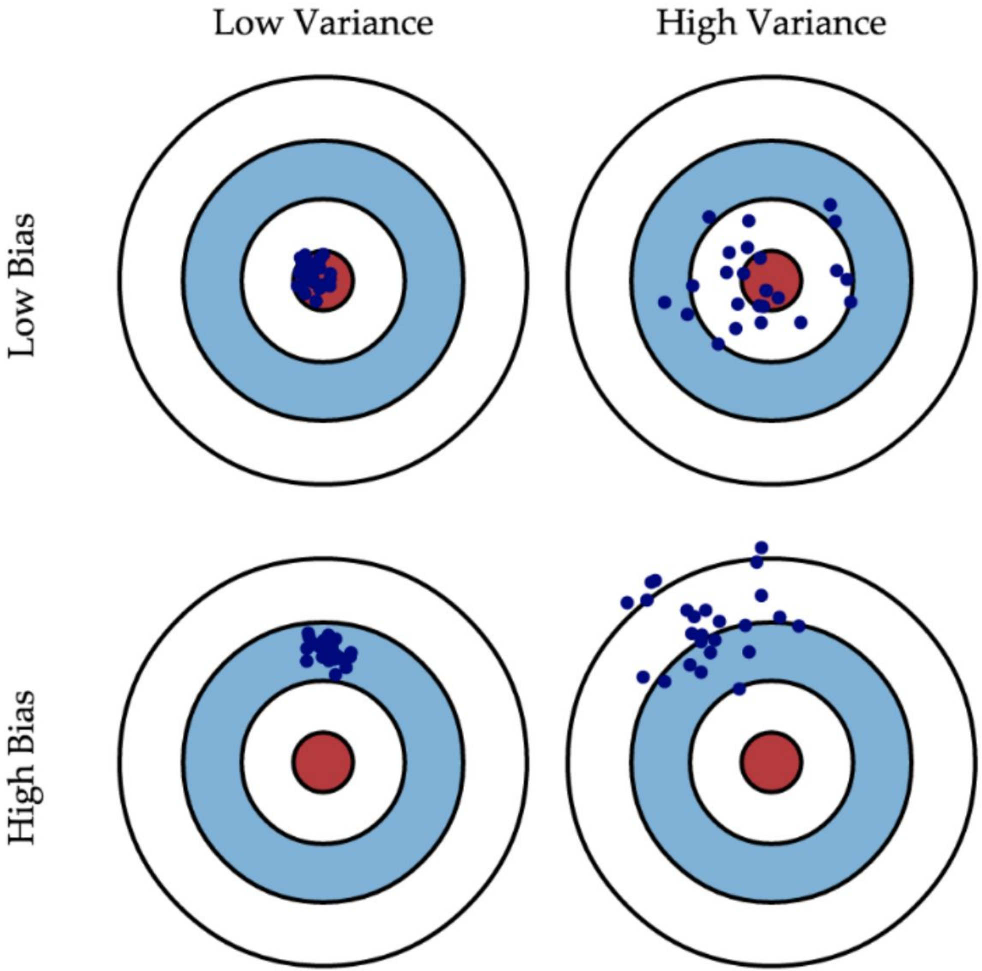
Recap: ensembling methods as of now

1. Bagging.
2. Random subspace method (RSM).
3. Bagging + RSM + Decision trees = Random Forest.
4. Blending.
5. Stacking.

Bias-Variance tradeoff

Bias-variance tradeoff




Low Variance
High Variance
Low Bias
High Bias

Bias-variance decomposition derivation

Bias-variance decomposition

The dataset $X = (x_i, y_i)_{i=1}^{\ell}$ with $y_i \in \mathbb{R}$

for regression problem.

Denote loss function $L(y, a) = \big(y - a(x)\big)^2$.

The empirical risk takes form:

$$R(a) = \mathbb{E}_{x,y}\Big[\big(y - a(x)\big)^2\Big] = \int_{\mathbb{X}}\int_{\mathbb{Y}} p(x, y)\big(y - a(x)\big)^2 dx dy.$$

Bias-variance decomposition

Let's show that

$$a_*(x) = \mathbb{E}[y \,|\, x] = \int_{\mathbb{Y}} y p(y \,|\, x) dy = \arg\min_a R(a).$$

$$L(y, a(x)) = (y - a(x))^2 = (y - \mathbb{E}(y \,|\, x) + \mathbb{E}(y \,|\, x) - a(x))^2 =$$
$$= (y - \mathbb{E}(y \,|\, x))^2 + 2\big(y - \mathbb{E}(y \,|\, x)\big)\big(\mathbb{E}(y \,|\, x) - a(x)\big) + (\mathbb{E}(y \,|\, x) - a(x))^2.$$

Returning to the risk estimation:

$$\begin{aligned} R(a) &= \mathbb{E}_{x,y} L(y, a(x)) = \\ &= \mathbb{E}_{x,y}(y - \mathbb{E}(y \,|\, x))^2 + \mathbb{E}_{x,y}(\mathbb{E}(y \,|\, x) - a(x))^2 + \\ &+ 2\mathbb{E}_{x,y}\big(y - \mathbb{E}(y \,|\, x)\big)\big(\mathbb{E}(y \,|\, x) - a(x)\big). \end{aligned}$$

Focus on the last term:

$$R(a) = \mathbb{E}_{x,y} L(y, a(x)) =$$
$$= \mathbb{E}_{x,y}(y - \mathbb{E}(y \,|\, x))^2 + \mathbb{E}_{x,y}(\mathbb{E}(y \,|\, x) - a(x))^2 +$$
$$+ 2\mathbb{E}_{x,y}\big(y - \mathbb{E}(y \,|\, x)\big)\big(\mathbb{E}(y \,|\, x) - a(x)\big).$$

Does not depend on y

$$\mathbb{E}_x \mathbb{E}_y \Big[\big(y - \mathbb{E}(y \,|\, x)\big) \boxed{\big(\mathbb{E}(y \,|\, x) - a(x)\big)} \,\Big|\, x \Big] =$$
$$= \mathbb{E}_x \Big(\big(\mathbb{E}(y \,|\, x) - a(x)\big) \mathbb{E}_y \Big[\big(y - \mathbb{E}(y \,|\, x)\big) \,\Big|\, x \Big] \Big) =$$
$$= \mathbb{E}_x \Big(\big(\mathbb{E}(y \,|\, x) - a(x)\big) \big(\mathbb{E}(y \,|\, x) - \mathbb{E}(y \,|\, x)\big) \Big) =$$
$$= 0$$

Focus on the last term:

$$
\begin{aligned}
R(a) &= \mathbb{E}_{x,y} L(y, a(x)) = \\
&= \mathbb{E}_{x,y}(y - \mathbb{E}(y \mid x))^2 + \mathbb{E}_{x,y}(\mathbb{E}(y \mid x) - a(x))^2 + \\
&\cancel{+ 2\mathbb{E}_{x,y}\big(y - \mathbb{E}(y \mid x)\big)\big(\mathbb{E}(y \mid x) - a(x)\big).} \rightarrow 0
\end{aligned}
$$

$$
\begin{aligned}
&\mathbb{E}_x \mathbb{E}_y \Big[\big(y - \mathbb{E}(y \mid x)\big)\big(\mathbb{E}(y \mid x) - a(x)\big) \mid x \Big] = \\
&= \mathbb{E}_x \Big(\big(\mathbb{E}(y \mid x) - a(x)\big) \mathbb{E}_y \Big[\big(y - \mathbb{E}(y \mid x)\big) \mid x \Big] \Big) = \\
&= \mathbb{E}_x \Big(\big(\mathbb{E}(y \mid x) - a(x)\big)\big(\mathbb{E}(y \mid x) - \mathbb{E}(y \mid x)\big) \Big) = \\
&= 0
\end{aligned}
$$

So the risk takes form:

$$R(a) = \boxed{\mathbb{E}_{x,y}(y - \mathbb{E}(y \mid x))^2} + \mathbb{E}_{x,y}(\mathbb{E}(y \mid x) - a(x))^2.$$

Does not depend on a(x)

The minimum is reached when $a(x) = \mathbb{E}(y \mid x).$

So the optimal regression model with square loss is

$$a_*(x) = \mathbb{E}(y \mid x) = \int_{\mathbb{Y}} yp(y \mid x)dy.$$

Denote $\mu : (\mathbb{X} \times \mathbb{Y})^\ell \to \mathcal{A}$, where $\mathcal{A}$ is some family of algorithms.

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So $L(\mu) = \mathbb{E}_X\left[\mathbb{E}_{x,y}\left[\left(y - \mu(X)(x)\right)^2\right]\right]$, where X dataset.

In further slides (x) is omitted!

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If X is fixed, then

$$\mathbb{E}_{x,y}\left[\left(y - \mu(X)\right)^2\right] = \mathbb{E}_{x,y}\left[\left(y - \mathbb{E}[y \mid x]\right)^2\right] + \mathbb{E}_{x,y}\left[\left(\mathbb{E}[y \mid x] - \mu(X)\right)^2\right].$$

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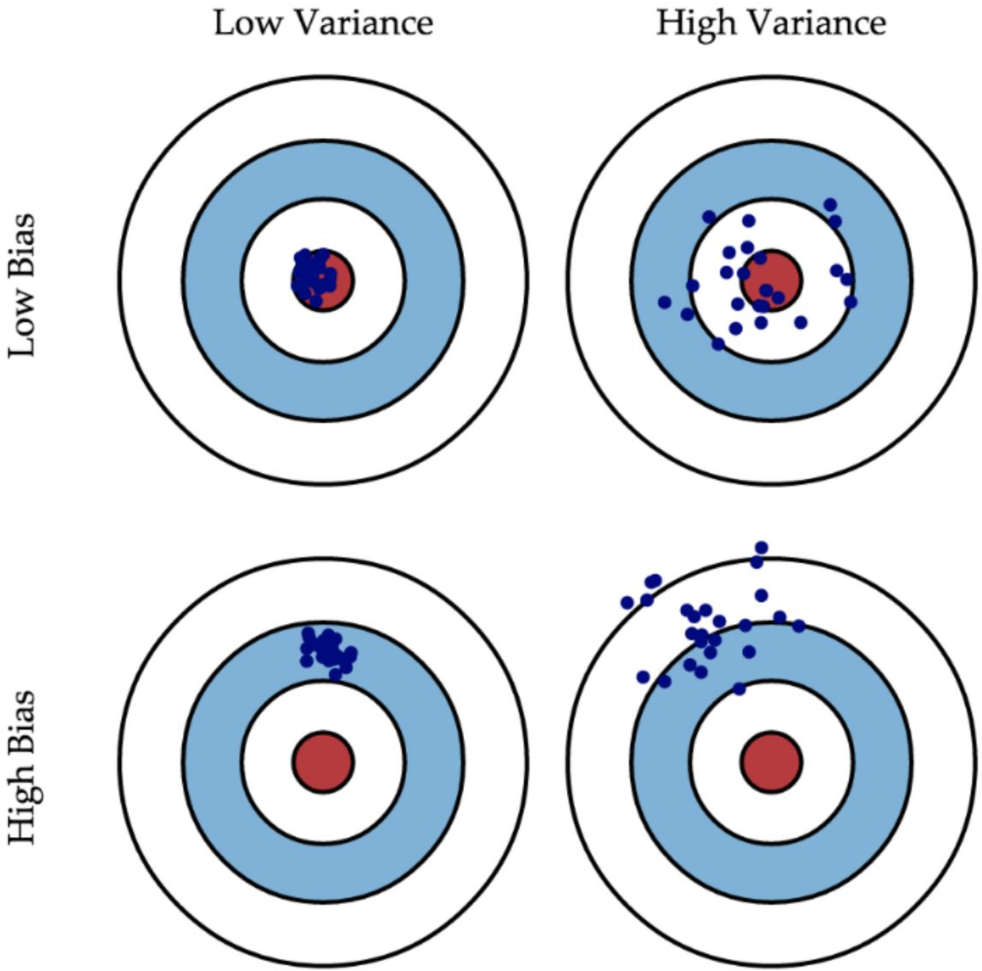
Let's combine the latter equations:

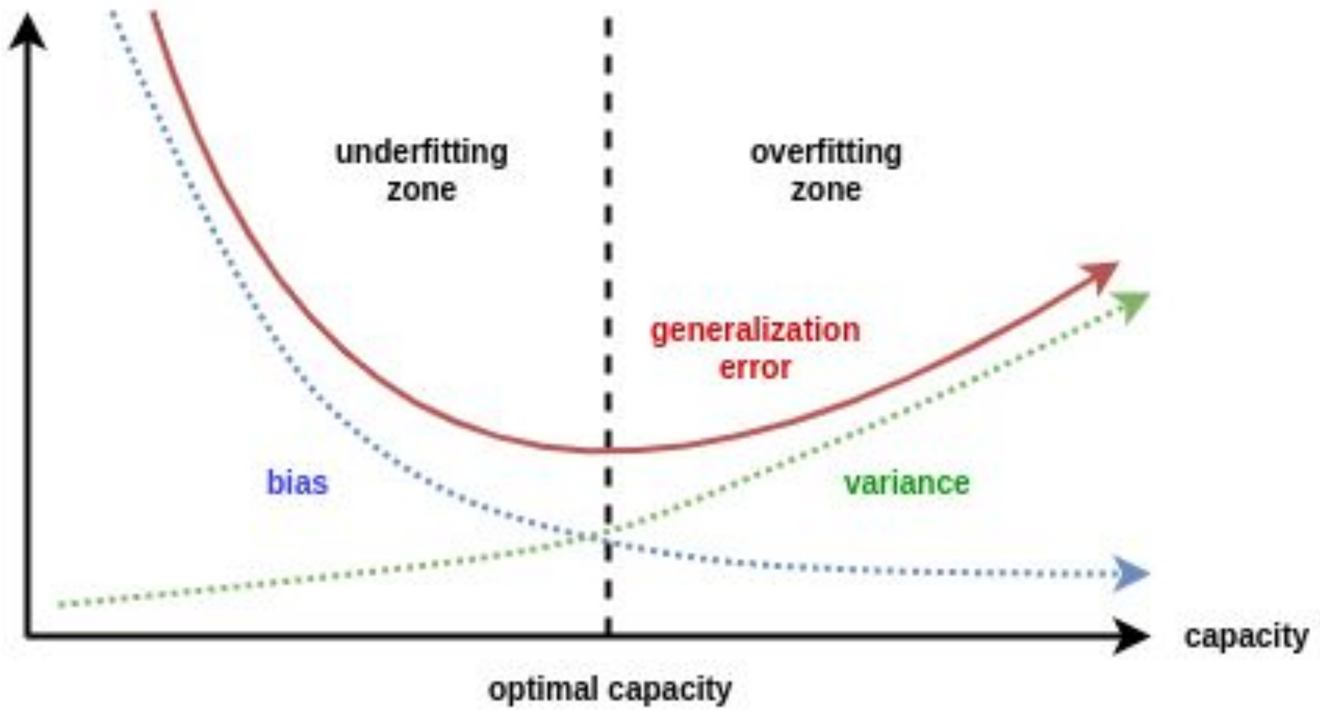
$$L(\mu) = \mathbb{E}_X\left[\underbrace{\mathbb{E}_{x,y}\left[\left(y - \mathbb{E}[y \mid x]\right)^2\right]}_{\text{Does not depend on X}} + \mathbb{E}_{x,y}\left[\left(\mathbb{E}[y \mid x] - \mu(X)\right)^2\right]\right]$$

$$L(\mu) = \underbrace{\mathbb{E}_{x,y}\left[\left(y - \mathbb{E}[y \mid x]\right)^2\right]}_{\text{noise}} +$$

$$+ \underbrace{\mathbb{E}_x\left[\left(\mathbb{E}_X\left[\mu(X)\right] - \mathbb{E}[y \mid x]\right)^2\right]}_{\text{bias}} + \underbrace{\mathbb{E}_x\left[\mathbb{E}_X\left[\left(\mu(X) - \mathbb{E}_X\left[\mu(X)\right]\right)^2\right]\right]}_{\text{variance}}.$$


Low Variance
High Variance
Low Bias
High Bias

Bias-variance tradeoff



$$L(\mu) = \underbrace{\mathbb{E}_{x,y}\left[\left(y - \mathbb{E}[y \mid x]\right)^2\right]}_{\text{noise}} +$$

$$+ \underbrace{\mathbb{E}_x\left[\left(\mathbb{E}_X\left[\mu(X)\right] - \mathbb{E}[y \mid x]\right)^2\right]}_{\text{bias}} + \underbrace{\mathbb{E}_x\left[\mathbb{E}_X\left[\left(\mu(X) - \mathbb{E}_X\left[\mu(X)\right]\right)^2\right]\right]}_{\text{variance}}.$$

This exact form of bias-variance decomposition is correct for square loss in regression.

However, it is much more general. See extra materials for more exotic cases.

Q & A

Appendix
(continue from slide 17)

$$L(\mu) = \mathbb{E}_X\Big[\underbrace{\mathbb{E}_{x,y}\Big[\big(y - \mathbb{E}[y \mid x]\big)^2\Big]}_{\text{Does not depend on X}} + \mathbb{E}_{x,y}\Big[\big(\mathbb{E}[y \mid x] - \mu(X)\big)^2\Big]\Big] =$$

$$L(\mu) = \mathbb{E}_X\left[\underbrace{\mathbb{E}_{x,y}\left[\left(y - \mathbb{E}[y \,|\, x]\right)^2\right]}_{\text{Does not depend on X}} + \mathbb{E}_{x,y}\left[\left(\mathbb{E}[y \,|\, x] - \mu(X)\right)^2\right]\right] =$$

$$= \mathbb{E}_{x,y}\left[\left(y - \mathbb{E}[y \,|\, x]\right)^2\right] + \mathbb{E}_{x,y}\left[\mathbb{E}_X\left[\left(\mathbb{E}[y \,|\, x] - \mu(X)\right)^2\right]\right].$$

$$L(\mu) = \mathbb{E}_X\left[\mathbb{E}_{x,y}\left[\left(y - \mathbb{E}[y \mid x]\right)^2\right] + \mathbb{E}_{x,y}\left[\left(\mathbb{E}[y \mid x] - \mu(X)\right)^2\right]\right] =$$

$$= \mathbb{E}_{x,y}\left[\left(y - \mathbb{E}[y \mid x]\right)^2\right] + \boxed{\mathbb{E}_{x,y}\left[\mathbb{E}_X\left[\left(\mathbb{E}[y \mid x] - \mu(X)\right)^2\right]\right]}.$$

Focus on the second term:

$$L(\mu) = \mathbb{E}_X\left[\mathbb{E}_{x,y}\left[\left(y - \mathbb{E}[y \mid x]\right)^2\right] + \mathbb{E}_{x,y}\left[\left(\mathbb{E}[y \mid x] - \mu(X)\right)^2\right]\right] =$$

$$= \mathbb{E}_{x,y}\left[\left(y - \mathbb{E}[y \mid x]\right)^2\right] + \boxed{\mathbb{E}_{x,y}\left[\mathbb{E}_X\left[\left(\mathbb{E}[y \mid x] - \mu(X)\right)^2\right]\right]}.$$

Focus on the second term:

$$\mathbb{E}_{x,y}\left[\mathbb{E}_X\left[\left(\mathbb{E}[y \mid x] - \mu(X)\right)^2\right]\right] =$$

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Focus on the second term:

$$\mathbb{E}_{x,y}\left[\mathbb{E}_X\left[\left(\mathbb{E}[y \mid x] - \mu(X)\right)^2\right]\right] =$$

$$= \mathbb{E}_{x,y}\left[\mathbb{E}_X\left[\left(\mathbb{E}[y \mid x] - \mathbb{E}_X\left[\mu(X)\right] + \mathbb{E}_X\left[\mu(X)\right] - \mu(X)\right)^2\right]\right]$$

$$\mathbb{E}_{x,y}\left[\mathbb{E}_X\left[\left(\mathbb{E}[y \mid x] - \mu(X)\right)^2\right]\right] =$$

$$= \mathbb{E}_{x,y}\left[\mathbb{E}_X\left[\left(\mathbb{E}[y \mid x] - \mathbb{E}_X\left[\mu(X)\right] + \mathbb{E}_X\left[\mu(X)\right] - \mu(X)\right)^2\right]\right] =$$

$$\mathbb{E}_{x,y}\left[\mathbb{E}_X\left[\left(\mathbb{E}[y\,|\,x]-\mu(X)\right)^2\right]\right]=$$

$$=\mathbb{E}_{x,y}\left[\mathbb{E}_X\left[\left(\mathbb{E}[y\,|\,x]-\mathbb{E}_X\left[\mu(X)\right]+\mathbb{E}_X\left[\mu(X)\right]-\mu(X)\right)^2\right]\right]=$$

$$=\mathbb{E}_{x,y}\left[\mathbb{E}_X\left[\underbrace{\left(\mathbb{E}[y\,|\,x]-\mathbb{E}_X\left[\mu(X)\right]\right)^2}\right]\right]+\mathbb{E}_{x,y}\left[\mathbb{E}_X\left[\left(\mathbb{E}_X\left[\mu(X)\right]-\mu(X)\right)^2\right]\right]+$$

$$+\,2\mathbb{E}_{x,y}\left[\mathbb{E}_X\left[\left(\mathbb{E}[y\,|\,x]-\mathbb{E}_X\left[\mu(X)\right]\right)\left(\mathbb{E}_X\left[\mu(X)\right]-\mu(X)\right)\right]\right].$$

$$
\begin{aligned}
&\mathbb{E}_{x,y}\left[\mathbb{E}_X\left[\left(\mathbb{E}[y \mid x]-\mu(X)\right)^2\right]\right]= \\
&=\mathbb{E}_{x,y}\left[\mathbb{E}_X\left[\left(\mathbb{E}[y \mid x]-\mathbb{E}_X\left[\mu(X)\right]+\mathbb{E}_X\left[\mu(X)\right]-\mu(X)\right)^2\right]\right]= \\
&=\mathbb{E}_{x,y}\left[\mathbb{E}_X\left[\underbrace{\left(\mathbb{E}[y \mid x]-\mathbb{E}_X\left[\mu(X)\right]\right)^2}_{\text{Does not depend on X}}\right]\right]+\mathbb{E}_{x,y}\left[\mathbb{E}_X\left[\left(\mathbb{E}_X\left[\mu(X)\right]-\mu(X)\right)^2\right]\right]+ \\
&\qquad +2\mathbb{E}_{x,y}\left[\mathbb{E}_X\left[\left(\mathbb{E}[y \mid x]-\mathbb{E}_X\left[\mu(X)\right]\right)\left(\mathbb{E}_X\left[\mu(X)\right]-\mu(X)\right)\right]\right].
\end{aligned}
$$

$$\mathbb{E}_{x,y}\left[\mathbb{E}_X\left[\left(\mathbb{E}[y\,|\,x] - \mu(X)\right)^2\right]\right] =$$

$$= \mathbb{E}_{x,y}\left[\mathbb{E}_X\left[\left(\mathbb{E}[y\,|\,x] - \mathbb{E}_X\left[\mu(X)\right] + \mathbb{E}_X\left[\mu(X)\right] - \mu(X)\right)^2\right]\right] =$$

$$= \mathbb{E}_{x,y}\left[\mathbb{E}_X\left[\underbrace{\left(\mathbb{E}[y\,|\,x] - \mathbb{E}_X\left[\mu(X)\right]\right)^2}_{\text{Does not depend on X}}\right]\right] + \mathbb{E}_{x,y}\left[\mathbb{E}_X\left[\left(\mathbb{E}_X\left[\mu(X)\right] - \mu(X)\right)^2\right]\right] +$$

$$+ 2\mathbb{E}_{x,y}\left[\mathbb{E}_X\left[\left(\mathbb{E}[y\,|\,x] - \mathbb{E}_X\left[\mu(X)\right]\right)\left(\mathbb{E}_X\left[\mu(X)\right] - \mu(X)\right)\right]\right].$$

Just a bit further, we are almost there

$$\mathbb{E}_{x,y}\left[\mathbb{E}_X\left[\left(\mathbb{E}[y\,|\,x]-\mu(X)\right)^2\right]\right]=$$

$$=\mathbb{E}_{x,y}\left[\mathbb{E}_X\left[\left(\mathbb{E}[y\,|\,x]-\mathbb{E}_X\left[\mu(X)\right]+\mathbb{E}_X\left[\mu(X)\right]-\mu(X)\right)^2\right]\right]=$$

$$=\mathbb{E}_{x,y}\left[\mathbb{E}_X\left[\left(\mathbb{E}[y\,|\,x]-\mathbb{E}_X\left[\mu(X)\right]\right)^2\right]\right]+\mathbb{E}_{x,y}\left[\mathbb{E}_X\left[\left(\mathbb{E}_X\left[\mu(X)\right]-\mu(X)\right)^2\right]\right]+$$

$$\boxed{+\,2\mathbb{E}_{x,y}\left[\mathbb{E}_X\left[\left(\mathbb{E}[y\,|\,x]-\mathbb{E}_X\left[\mu(X)\right]\right)\left(\mathbb{E}_X\left[\mu(X)\right]-\mu(X)\right)\right]\right]}.$$

Focus on this term

$$\mathbb{E}_X\left[\left(\mathbb{E}[y \mid x] - \mathbb{E}_X\left[\mu(X)\right]\right)\left(\mathbb{E}_X\left[\mu(X)\right] - \mu(X)\right)\right] =$$

$$\mathbb{E}_X\Big[\big(\mathbb{E}[y\,|\,x] - \mathbb{E}_X\left[\mu(X)\right]\big)\big(\mathbb{E}_X\left[\mu(X)\right] - \mu(X)\big)\Big] =$$

$$= \big(\mathbb{E}[y\,|\,x] - \mathbb{E}_X\left[\mu(X)\right]\big)\mathbb{E}_X\Big[\mathbb{E}_X\left[\mu(X)\right] - \mu(X)\Big] =$$

$$\mathbb{E}_X\Big[\big(\mathbb{E}[y\,|\,x] - \mathbb{E}_X\left[\mu(X)\right]\big)\big(\mathbb{E}_X\left[\mu(X)\right] - \mu(X)\big)\Big] =$$

$$= \big(\mathbb{E}[y\,|\,x] - \mathbb{E}_X\left[\mu(X)\right]\big)\mathbb{E}_X\Big[\mathbb{E}_X\left[\mu(X)\right] - \mu(X)\Big] =$$

$$= \big(\mathbb{E}[y\,|\,x] - \mathbb{E}_X\left[\mu(X)\right]\big)\Big[\mathbb{E}_X\left[\mu(X)\right] - \mathbb{E}_X\left[\mu(X)\right]\Big] =$$

$$
\begin{aligned}
\mathbb{E}_X\Big[\big(\mathbb{E}[y \mid x] - \mathbb{E}_X\left[\mu(X)\right]\big)\left(\mathbb{E}_X\left[\mu(X)\right] - \mu(X)\right)\Big] &= \\
&= \big(\mathbb{E}[y \mid x] - \mathbb{E}_X\left[\mu(X)\right]\big)\mathbb{E}_X\Big[\mathbb{E}_X\left[\mu(X)\right] - \mu(X)\Big] = \\
&= \big(\mathbb{E}[y \mid x] - \mathbb{E}_X\left[\mu(X)\right]\big)\Big[\mathbb{E}_X\left[\mu(X)\right] - \mathbb{E}_X\left[\mu(X)\right]\Big] = \\
&= 0.
\end{aligned}
$$

$$\mathbb{E}_{x,y}\left[\mathbb{E}_X\left[\left(\mathbb{E}[y \mid x] - \mu(X)\right)^2\right]\right] =$$

$$= \mathbb{E}_{x,y}\left[\mathbb{E}_X\left[\left(\mathbb{E}[y \mid x] - \mathbb{E}_X\left[\mu(X)\right] + \mathbb{E}_X\left[\mu(X)\right] - \mu(X)\right)^2\right]\right] =$$

$$= \mathbb{E}_{x,y}\left[\mathbb{E}_X\left[\left(\mathbb{E}[y \mid x] - \mathbb{E}_X\left[\mu(X)\right]\right)^2\right]\right] + \mathbb{E}_{x,y}\left[\mathbb{E}_X\left[\left(\mathbb{E}_X\left[\mu(X)\right] - \mu(X)\right)^2\right]\right] +$$

$$+ \cancel{2\mathbb{E}_{x,y}\left[\mathbb{E}_X\left[\left(\mathbb{E}[y \mid x] - \mathbb{E}_X\left[\mu(X)\right]\right)\left(\mathbb{E}_X\left[\mu(X)\right] - \mu(X)\right)\right]\right]} \rightarrow 0.$$