STATISTICAL MACHINE LEARNING

— Squared Error Decomposition

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Let

$$f_*(X) = \mathbb{E}Y|X$$

be the regression function and

$$\overline{f}(X) = \mathbb{E}_{\mathcal{D}} \hat{f}(X)$$

be the average over the training distribution of the procedure \hat{f} . Then

$$R(\hat{f}) := \mathbb{E}_{\mathcal{D},Z}(Y - \hat{f}(X))^2 \tag{1}$$

$$= \mathbb{E}_{\mathcal{D},Z}(Y - f_*(X) + f_*(X) - \overline{f}(X) + \overline{f}(X) - \hat{f}(X))^2$$
(2)

$$= \mathbb{E}_{\mathcal{D},Z}(Y - f_*(X))^2 + \mathbb{E}_{\mathcal{D},Z}(f_*(X) - \overline{f}(X))^2 + \mathbb{E}_{\mathcal{D},Z}(\overline{f}(X) - \hat{f}(X))^2 +$$
(3)

$$\mathbb{E}_{\mathcal{D},Z}(Y - f_*(X))(f_*(X) - \overline{f}(X)) + \mathbb{E}_{\mathcal{D},Z}(f_*(X) - \overline{f}(X))(\overline{f}(X) - \hat{f}(X)) + \tag{4}$$

$$+ \mathbb{E}_{\mathcal{D},Z}(Y - f_*(X))(\overline{f}(X) - \hat{f}(X)) \tag{5}$$

$$= \sigma^2 + B + V + \tag{6}$$

$$(I) + (II) + \tag{7}$$

$$+(III)$$
 (8)

Both σ^2 and B do not depend on \mathcal{D} , so the integration is only with respect to Z. Hence

$$\sigma^2 = \mathbb{E}_Z(Y - f_*(X))^2 = \mathbb{E}_X \mathbb{E}_{Y|X} (Y - f_*(X))^2.$$

Also, there is no Y in B, hence we are only integrating with respect to the marginal of X

$$\mathbb{E}_{\mathcal{D},Z}(f_*(X) - \overline{f}(X))^2 = \mathbb{E}_X(f_*(X) - \overline{f}(X))^2 = \int (f_*(X) - \overline{f}(X))^2 d\mathbb{P}_X,$$

and similarly

$$\mathbb{E}_{\mathcal{D},Z}(\overline{f}(X) - \hat{f}(X))^2 = \mathbb{E}_Z \mathbb{V}\hat{f}(X) = \int \mathbb{V}\hat{f}(X)d\mathbb{P}_X.$$

The cross terms can be seen to be zero

$$(I) = \mathbb{E}_{\mathcal{D},Z}(Y - f_*(X))(f_*(X) - \overline{f}(X)) = \mathbb{E}_{\mathcal{D}}\mathbb{E}_X(f_*(X) - \overline{f}(X))\mathbb{E}_{Y|X}(Y - f_*(X)) = 0,$$

$$(II) = \mathbb{E}_{\mathcal{D},Z}(f_*(X) - \overline{f}(X))(\overline{f}(X) - \hat{f}(X)) = \mathbb{E}_Z(f_*(X) - \overline{f}(X))\mathbb{E}_{\mathcal{D}}(\overline{f}(X) - \hat{f}(X)) = 0,$$

and

$$(III) = \mathbb{E}_{\mathcal{D},Z}(Y - f_*(X))(\overline{f}(X) - \hat{f}(X)) = \mathbb{E}_{\mathcal{D}}\mathbb{E}_X(\overline{f}(X) - \hat{f}(X))\mathbb{E}_{Y|X}(Y - f_*(X)) = 0.$$