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Bias Variance Tradeoff

Consider a training set $S = \{(x_1, y_1), (x_2, y_2), ..., (x_n, y_n)\}$ and the random variable y which we cant to model it.

We asumming there is a function $f(x)$ that:

$$\boxed{y = f(x) + \epsilon}$$

with $e \sim D(0, \sigma^2)$.

When we training a model we want to find a function $\hat{f}(x|S)$ which approximates $f(x)$. Note $f(x)$ is deterministic and $\hat{f}(x|S)$ depends of the model chosen and its hyperparameters among others and for that it is a random variable.

The error of the aproximation is:

$$\boxed{\mathbb{E}\left[(y - \hat{f}(x))^2|S\right]}$$

We will developed every term.

$$\mathbb{E}\left[(y - \hat{f}(x))^2|S\right] = \mathbb{E}\left[y^2 - 2 \cdot y \cdot \hat{f}(x) + (\hat{f}(x))^2|S\right] = \mathbb{E}\left[y^2|S\right] - 2 \cdot \mathbb{E}\left[y \cdot \hat{f}(x)|S\right] + \mathbb{E}\left[(\hat{f}(x))^2|S\right]$$

$\Rightarrow$

$$\boxed{\mathbb{E}\left[(y - \hat{f}(x))^2|S\right] = \mathbb{E}\left[y^2|S\right] - 2 \cdot \mathbb{E}\left[y \cdot \hat{f}(x)|S\right] + \mathbb{E}\left[(\hat{f}(x))^2|S\right]} \quad (1)$$

Also we have:

$$\mathbb{V}\left[\hat{f}(x)|S\right] = \mathbb{E}\left[(\hat{f}(x))^2|S\right] - \left(\mathbb{E}\left[\hat{f}(x)|S\right]\right)^2$$

$\Rightarrow$

$$\boxed{\mathbb{E}\left[(\hat{f}(x))^2|S\right] = \mathbb{V}\left[\hat{f}(x)|S\right] + \left(\mathbb{E}\left[\hat{f}(x)|S\right]\right)^2} \quad (2)$$

Combining (1) and (2) we have:

$$\boxed{\mathbb{E}\left[(y-\hat{f}(x))^2|S\right] = \mathbb{E}\left[y^2|S\right] - 2\cdot\mathbb{E}\left[y\cdot\hat{f}(x)|S\right] + \mathbb{V}\left[\hat{f}(x)|S\right] + \left(\mathbb{E}\left[\hat{f}(x)|S\right]\right)^2} \quad (3)$$

Now:

$$\mathbb{E}\left[y^2|S\right] = \mathbb{E}\left[(f(x)+\epsilon)^2|S\right] = \mathbb{E}\left[f(x)^2 + 2\cdot\epsilon\cdot f(x) + \epsilon^2|S\right]$$

$$= \mathbb{E}\left[f(x)^2|S\right] + \mathbb{E}\left[2\cdot\epsilon\cdot f(x)|S\right] + \mathbb{E}\left[\epsilon^2|S\right] = f(x)^2 + 2\cdot f(x)\cdot\mathbb{E}\left[\epsilon|S\right] + \mathbb{E}\left[\epsilon^2|S\right]$$

$$= f(x)^2 + 2\cdot f(x)\cdot 0 + \mathbb{V}\left[\epsilon|S\right] + \left(\mathbb{E}\left[\epsilon|S\right]\right)^2 = f(x)^2 + \sigma^2$$

$\Rightarrow$

$$\mathbb{E}\left[y^2|S\right] = f(x)^2 + \sigma^2$$

Replacing this in (3):

$$\boxed{\mathbb{E}\left[(y-\hat{f}(x))^2|S\right] = f(x)^2 + \sigma^2 - 2\cdot\mathbb{E}\left[y\cdot\hat{f}(x)|S\right] + \mathbb{V}\left[\hat{f}(x)|S\right] + \left(\mathbb{E}\left[\hat{f}(x)|S\right]\right)^2} \quad (4)$$

On the other hand:

$$\mathbb{E}\left[y\cdot\hat{f}(x)|S\right] = \mathbb{E}\left[(f(x)+\epsilon)\cdot\hat{f}(x)|S\right] = \mathbb{E}\left[f(x)\cdot\hat{f}(x)|S\right] + \mathbb{E}\left[\epsilon\cdot\hat{f}(x)|S\right]$$

$$\overset{\hat{f}(x)\text{ and }\epsilon\text{ are independent}}{=} f(x)\cdot\mathbb{E}\left[\hat{f}(x)|S\right] + \mathbb{E}\left[\epsilon|S\right]\cdot\mathbb{E}\left[\hat{f}(x)|S\right]$$

$$= f(x)\cdot\mathbb{E}\left[\hat{f}(x)|S\right] + 0\cdot\mathbb{E}\left[\hat{f}(x)|S\right] = f(x)\cdot\mathbb{E}\left[\hat{f}(x)|S\right]$$

$\Rightarrow$

$$\mathbb{E}\left[y\cdot\hat{f}(x)|S\right] = f(x)\cdot\mathbb{E}\left[\hat{f}(x)|S\right]$$

Replacing this in (4) we have that:

$$\mathbb{E}\left[(y-\hat{f}(x))^2|S\right] = f(x)^2 + \sigma^2 - 2\cdot f(x)\cdot\mathbb{E}\left[\hat{f}(x)|S\right] + \mathbb{V}\left[\hat{f}(x)|S\right] + \left(\mathbb{E}\left[\hat{f}(x)|S\right]\right)^2$$

$$= \left[f(x)^2 - 2\cdot f(x)\cdot\mathbb{E}\left[\hat{f}(x)|S\right] + \left(\mathbb{E}\left[\hat{f}(x)|S\right]\right)^2\right] + \mathbb{V}\left[\hat{f}(x)|S\right] + \sigma^2$$

$$= \left(f(x) - \mathbb{E}\left[\hat{f}(x)|S\right]\right)^2 + \mathbb{V}\left[\hat{f}(x)|S\right] + \sigma^2$$

$\Rightarrow$

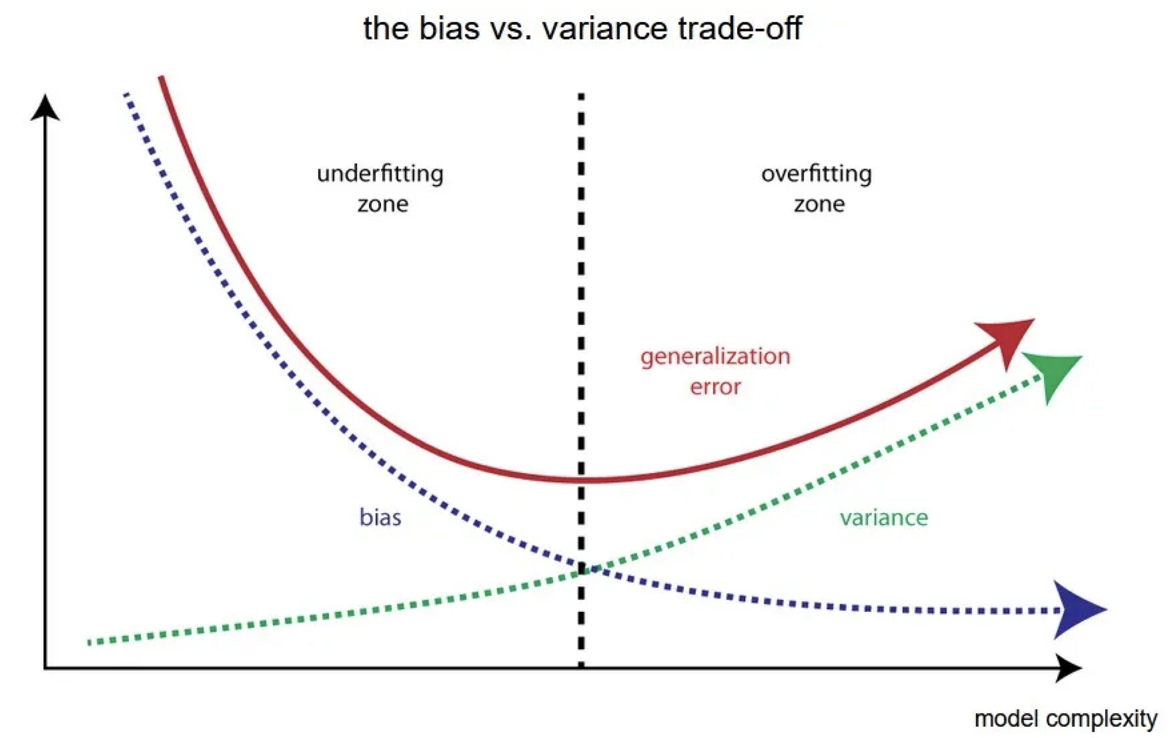
$$\mathbb{E}\left[(y-\hat{f}(x))^2|S\right] = \left(f(x) - \mathbb{E}\left[\hat{f}(x)|S\right]\right)^2 + \mathbb{V}\left[\hat{f}(x)|S\right] + \sigma^2$$

$\Rightarrow$

$$\mathbb{E}\left[(y - \hat{f}(x))^2 | S\right] = bias^2 + variance + \sigma^2$$

We can consider:

- $bias$ = error in training set.
- $variance$ = error in test set.



How to solve underfitting?

- Try more complex models.
- Increase the number of parameters.

How to solve overfitting?

- Try more simple models.
- Reduce the number of parameters.
- Check if the problem is imbalanced (classification or regression).
