Machine Learning I

Supervised learning framework - Optimal predictions

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Optimal prediction function

$$\boxed{f = \operatorname*{argmin}_{h:\mathcal{X}\to\mathcal{Y}} E_{\text{out}}(h)} \qquad \boxed{g = \operatorname*{argmin}_{h\in\mathcal{H}} E_{\text{in}}(h)}$$

Recall that the **optimal prediction function** is given by

$$f = \operatorname*{argmin}_{h:\mathcal{X}\to\mathcal{Y}} \underbrace{\mathbb{E}_x \left[E_{\text{out}}(h, x)\right]}_{E_{\text{out}}(h)}, \tag{1}$$

where

$$E_{\text{out}}(h, x) = \mathbb{E}_{y|x}[L(y, h(x))|x].$$

and $L(\cdot, \cdot)$ is the loss function.

It sufficed to minimize the error pointwise, i.e. compute

$$f(x) = \operatorname*{argmin}_{h:\mathcal{X}\to\mathcal{Y}} E_{\text{out}}(h, x), \tag{2}$$

for all $x \in \mathcal{X}$.

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Optimal predictions in regression (squared error loss)

With the squared error loss function $L(y, \hat{y}) = (y - \hat{y})^2$, the optimal prediction function is given by

$$
\begin{aligned}
f(x) &= \operatorname*{argmin}_{h:\mathcal{X}\to\mathcal{Y}} \mathbb{E}_{y|x}[(y - h(x))^2|x] && (3) \\
&= \mathbb{E}_{y|x}[y|x], && (4)
\end{aligned}
$$

i.e. the conditional expectation, also known as the **regression function**.

In other words, when *best is measured by expected squared error*, the best prediction for y at any point x is the conditional expectation at x.

Optimal predictions in regression (squared error loss)

$$
\begin{aligned}
& E_{\text{out}}(h, x) && (5)\\
&= \mathbb{E}_{y|x}[(y - h(x))^2 | x] && (6)\\
&= \mathbb{E}[y^2 - 2yh(x) + h(x)^2 | x] && (7)\\
&= \mathbb{E}[y^2|x] - 2h(x)\mathbb{E}[y|x] + h(x)^2 && (8)\\
&= \mathrm{Var}(y|x) + (\mathbb{E}[y|x])^2 - 2h(x)\mathbb{E}[y|x] + h(x)^2 && (9)\\
&= \mathrm{Var}(y|x) + (\mathbb{E}[y|x] - h(x))^2 && (10)
\end{aligned}
$$

- The second term is non-negative, and will be equal to zero if $h(x) = \mathbb{E}[y|x]$.
- The first term corresponds to the inherent unpredictability, or noise, of the output, and is called the **Bayes error**. It is the smallest error any learning algorithm can achieve.

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Optimal predictions in regression (zero-one loss)

For a multi-class classification problem with K categories, i.e. $y \in \mathcal{C} = \{C_1, \ldots, C_K\}$ and the zero-one loss function $L(y, \hat{y}) = \mathbb{1}\{y \neq \hat{y}\}$, the optimal prediction function is given by

$$f(x) = \operatorname*{argmin}_{h:\mathcal{X}\to\mathcal{C}} \mathbb{E}_{y|x}[\mathbb{1}\{y \neq h(x)\}|x] \tag{11}$$

$$= \operatorname*{argmax}_{h:\mathcal{X}\to\mathcal{C}} \mathbb{P}(y = h(x)|x). \tag{12}$$

The optimal classifier is called the **Bayes classifier**, which has the following error rate at x:

$$1 - \max_{k=1,\ldots,K} \mathbb{P}(y = C_k|x),$$

also called the **Bayes error rate**, which gives the lowest possible error rate that could be achieved <u>if we knew</u> $\mathbb{P}(y|x)$.

Optimal predictions in regression (zero-one loss)

$$
\begin{aligned}
E_{\text{out}}(h, x) &= \mathbb{E}_{y|x}[\mathbb{1}\{y \neq h(x)\}|x] \\
&= \sum_{k=1}^{K} \mathbb{1}\{C_k \neq h(x)\}\ \mathbb{P}(y = C_k|x) \\
&= \sum_{k: C_k \neq h(x)} 1 \times \mathbb{P}(y = C_k|x) + 0 \times \mathbb{P}(y = h(x)|x) \\
&= \sum_{k: C_k \neq h(x)} \mathbb{P}(y = C_k|x) \\
&= \sum_{k: C_k \neq h(x)} \mathbb{P}(y = C_k|x) + \mathbb{P}(y = h(x)|x) - \mathbb{P}(y = h(x)|x) \\
&= \sum_{k=1}^{K} \mathbb{P}(y = C_k|x) - \mathbb{P}(y = h(x)|x) \\
&= 1 - \mathbb{P}(y = h(x)|x).
\end{aligned}
$$

Optimal predictions in classification

Using the fundamental bridge, we can directly write

$$
\begin{aligned}
&\mathbb{E}_{y|x}[\mathbb{1}\{y \neq h(x)\}|x] \\
&= \mathbb{P}(y \neq h(x)|x) \\
&= 1 - \mathbb{P}(y = h(x)|x).
\end{aligned}
$$

In conclusion, we have

$$
\begin{aligned}
f(x) &= \operatorname*{argmin}_{h:\mathcal{X}\to\mathcal{C}} \mathbb{E}_{y|x}[\mathbb{1}\{y \neq h(x)\}|x] && (13) \\
&= \operatorname*{argmin}_{h:\mathcal{X}\to\mathcal{C}} 1 - \mathbb{P}(y = h(x)|x) && (14) \\
&= \operatorname*{argmax}_{h:\mathcal{X}\to\mathcal{C}} \mathbb{P}(y = h(x)|x). && (15)
\end{aligned}
$$

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Data distribution in regression

The data distribution $p_{x,y}$ is often **implicitly specified**, i.e. $p_{x,y}$ is not given explicitly. In regression, the following (additive error) data generating process is often considered:

$$y = f(x) + \varepsilon, \tag{16}$$

where

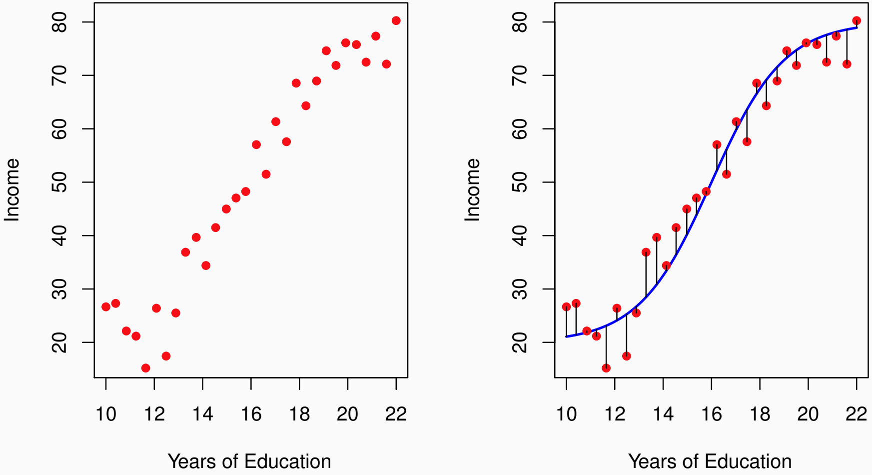
- $x \sim p_x$ (e.g. $p_x(x) = \frac{1}{2}$ for $x \in [-1, 1]$)
- f is a fixed unknown function (e.g. $f(x) = x^2$)
- ε is random noise, where
  - $\mathbb{E}[\varepsilon|x] = 0$
  - $\mathrm{Var}(\varepsilon|x) = \sigma^2$, with $\sigma \in [0, \infty)$.

Note that we have

- $\mathbb{E}[y|x] = f(x)$ and $\mathrm{Var}[y|x] = \sigma^2$

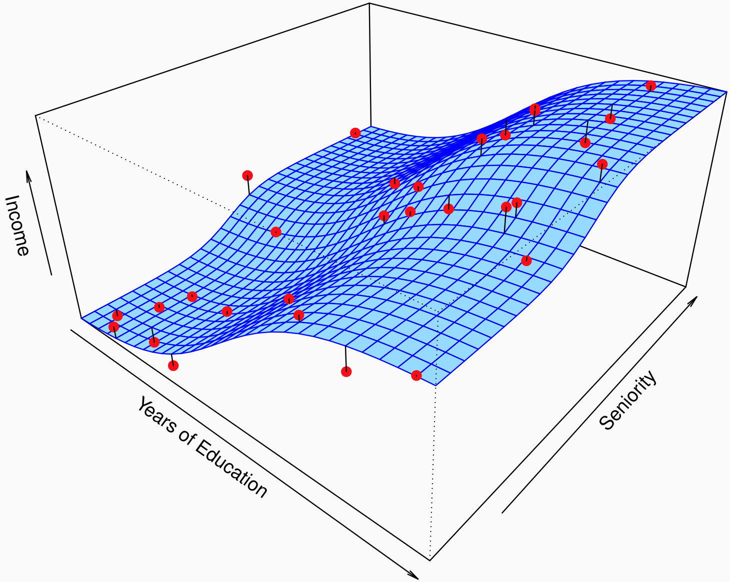
i.e. $p_{y|x}$ depends on x only through the conditional mean.

Data distribution in regression



$\rightarrow$ Try to visualize $p_{x,y}$

Data distribution in regression



Data distribution in classification

Using Bayes' rule, we can write

$$p(y|x) = \frac{p(x|y)p(y)}{p(x)} \propto p(x|y)p(y) \overset{y \text{ uniform}}{\propto} p(x|y)$$

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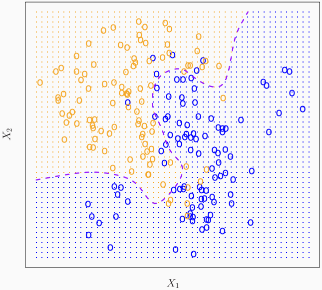

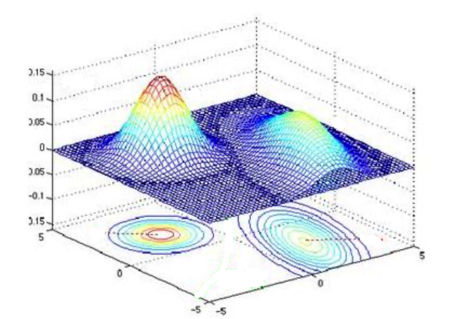

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The bias-variance decomposition

- Previously, we considered the **unrealistic scenario** where we know $p_{x,y}$. As a result, we were able to compute the optimal hypothesis/predictions for different loss functions.
- In practice, we only observe a **dataset** $\mathcal{D}$ where each data point is assumed to be an i.i.d. realization from $p_{x,y}$.
- Overly simple models underfit and complex models overfit. There is an **approximation-generalization** tradeoff:

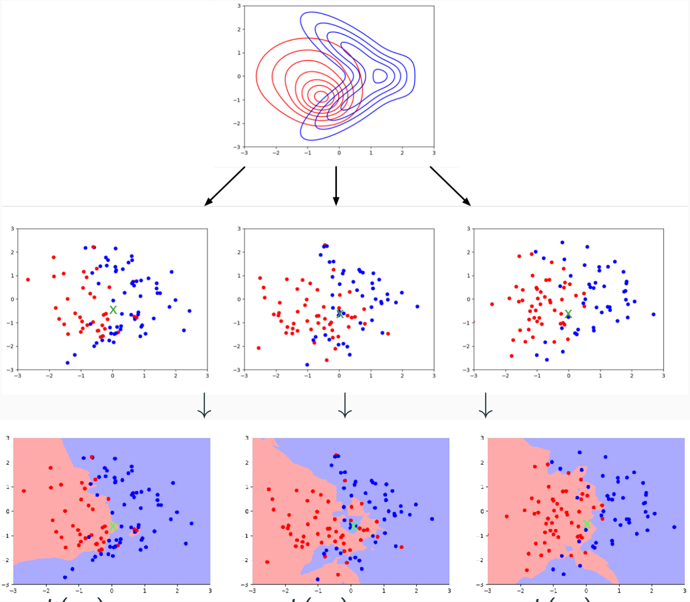
$$E_{\text{out}}(g) - E_{\text{out}}(f) = \underbrace{[E_{\text{out}}(g^*) - E_{\text{out}}(f)]}_{\text{Approximation error}} + \underbrace{[E_{\text{out}}(g) - E_{\text{out}}(g^*)]}_{\text{Estimation error}}$$

- The **bias-variance** decomposition allows to quantify this tradeoff for the **squared error** loss function.

An experiment

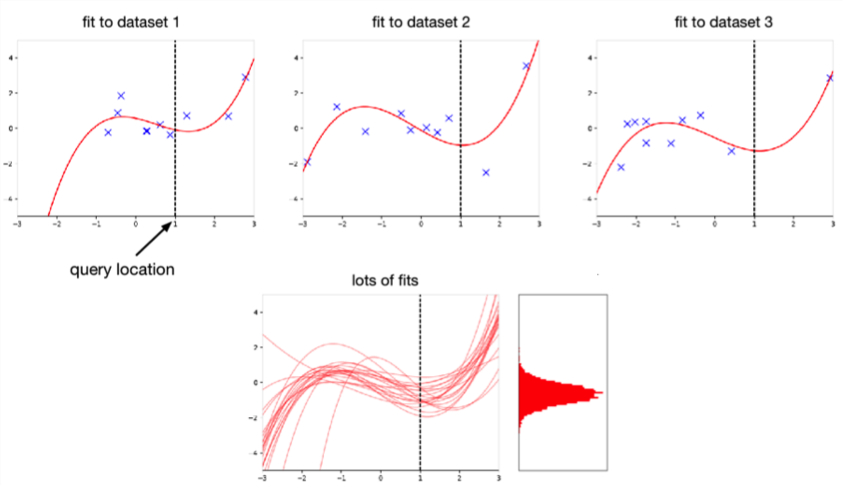
- Consider an experiment where we sample lots of training sets independently from $p_{x,y}$.
- Pick a fixed query point x_*.
- Let's run our learning algorithm on each training set, and compute its prediction $g(x_*)$ at the query point x_*.
- We can view $g(x_*)(= g_{\mathcal{D}}(x_*))$ as a random variable, where the randomness comes from the training set $\mathcal{D}$.

An experiment - Classification



$h(x_*) = $ ● $\quad h(x_*) = $ ● $\quad h(x_*) = $ ●

An experiment - Regression



An experiment (continued)

- Fix a query point x_*.
- Repeat:
  - Sample a dataset $\mathcal{D}$ i.i.d. from $p_{x,y}$
  - Run the learning algorithm on $\mathcal{D}$ to obtain g
  - Compute the prediction for x_*, i.e. $g(x_*)$
  - Sample the (true) output y_* from $p_{y|x}(\cdot|x = x_*)$
  - Compute the loss $L(y_*, g(x_*))$

$L(y_*, g(x_*))$ contains two sources of randomness: $\mathcal{D}$ and y_*. This gives a distribution over the loss at x_*.

An experiment (continued)

- Fix a query point x_*.
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$L(y_*, g(x_*))$ contains two sources of randomness: $\mathcal{D}$ and y_*. This gives a distribution over the loss at x_*.

Let us compute

$$\mathbb{E}_{\mathcal{D}}\left[\underbrace{\mathbb{E}_{y|x}\left[L(y, g(x))|x\right]}_{E_{\text{out}}(g,x)}\right]$$

for the squared error loss $L(y, g(x)) = (y - g(x))^2$.

The bias-variance decomposition

Previously, we proved that

$$E_{\text{out}}(g, x) = \mathbb{E}_{y|x}[(y - g(x))^2 | x] = \text{Var}(y|x) + (f(x) - g(x))^2,$$

where $f(x) = \mathbb{E}[y|x]$.

We can write

$$\begin{aligned} &\mathbb{E}_{\mathcal{D}}[E_{\text{out}}(g, x)] \\ &= ? \end{aligned}$$

The bias-variance decomposition

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where $f(x) = \mathbb{E}[y|x]$.

We can write

$$\begin{aligned}
&\mathbb{E}_{\mathcal{D}}[E_{\text{out}}(g, x)] \\
&= \text{Var}(y|x) + \mathbb{E}_{\mathcal{D}}[(f(x) - g(x))^2] \\
&= \text{Var}(y|x) + f(x)^2 - 2f(x)\mathbb{E}_{\mathcal{D}}[g(x)] + \mathbb{E}_{\mathcal{D}}[g(x)^2] \\
&= \text{Var}(y|x) + f(x)^2 - 2f(x)\mathbb{E}_{\mathcal{D}}[g(x)] + \text{Var}(g(x)) + \mathbb{E}_{\mathcal{D}}[g(x)]^2 \\
&= \underbrace{\text{Var}(y|x)}_{\text{Bayes error at } x} + \underbrace{(f(x) - \mathbb{E}_{\mathcal{D}}[g(x)])^2}_{\text{Bias at } x} + \underbrace{\text{Var}(g(x))}_{\text{Variance at } x}
\end{aligned}$$

The bias-variance decomposition

$$\mathbb{E}_{\mathcal{D},y|x}[(y-g(x))^2|x] = \underbrace{\mathrm{Var}(y|x)}_{\text{Bayes error at } x} + \underbrace{(f(x) - \mathbb{E}_{\mathcal{D}}[g(x)])^2}_{\text{Bias at } x} + \underbrace{\mathrm{Var}(g(x))}_{\text{Variance at } x}$$

We split the expected error at x into three terms:

- Bayes error: the inherent unpredictability of the output
- **bias**: how wrong the expected prediction is (underfitting)
- **variance**: the variability of the predictions (overfitting)

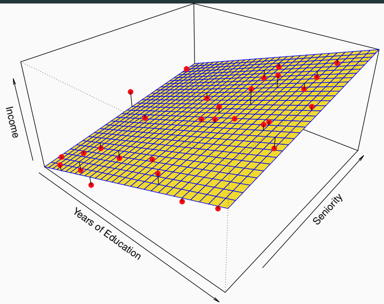
The bias-variance decomposition

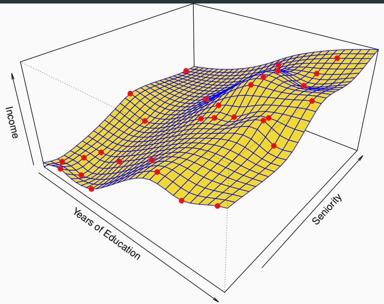
If we take the expectation with respect to x, we obtain

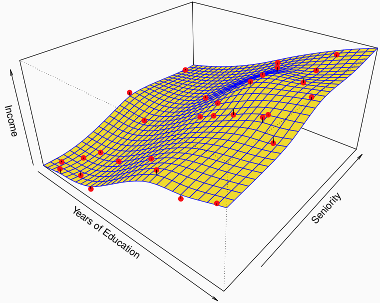
$$\begin{aligned}
&\mathbb{E}_{\mathcal{D},y,x}[(y - g(x))^2] \\
&= \underbrace{\mathrm{Var}(y)}_{\text{Bayes error}} + \underbrace{\mathbb{E}_x[(f(x) - \mathbb{E}_{\mathcal{D}}[g(x)])^2]}_{\text{Bias}} + \underbrace{\mathbb{E}_x[\mathrm{Var}(g(x))]}_{\text{Variance}}
\end{aligned}$$

While the analysis only applies to squared error, we often use "bias"/'variance" as synonyms for "underfitting"/"overfitting".

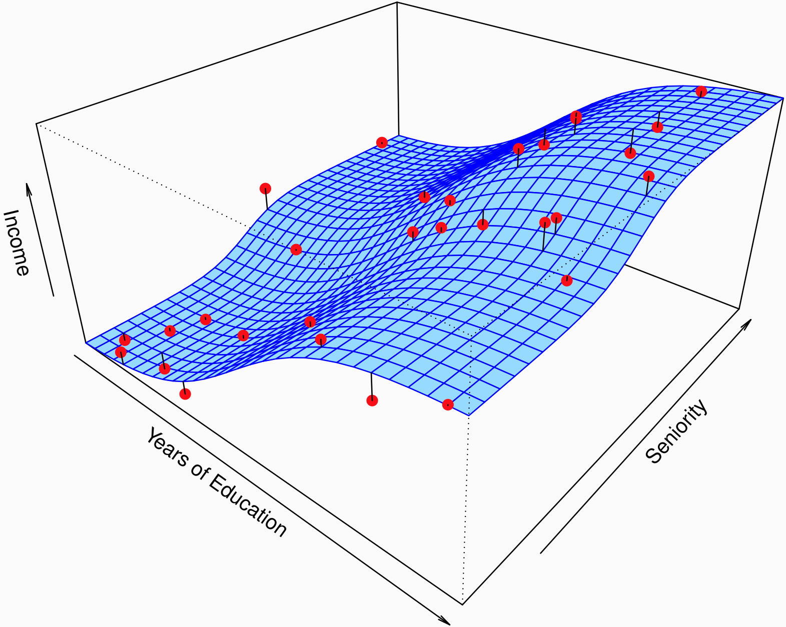
The bias-variance tradeoff



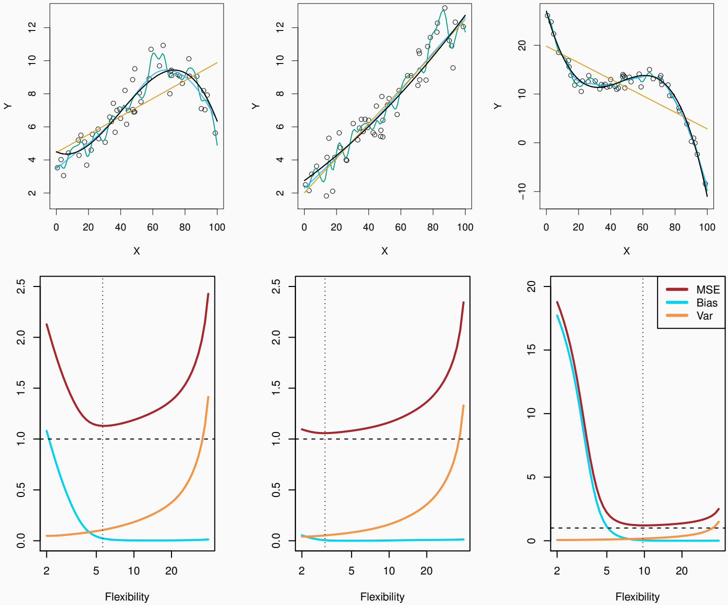




The bias-variance tradeoff



The bias-variance tradeoff



The bias-variance tradeoff

Throwing darts = predictions for each draw of a dataset