Machine Learning I

Supervised Learning: Bias and variance decomposition

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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:

$$y = f(x) + \varepsilon, \tag{1}$$

where

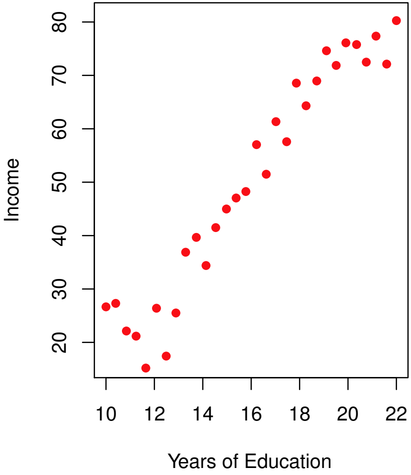
- $x \sim p_x$ (e.g. $p_x(x) = \frac{1}{2}$ for $x \in [-1, 1]$)
- f is a fixed unknown function (e.g. $f(x) = x^2$)
- ε is random noise, where
  - $\mathbb{E}[\varepsilon|x] = 0$
  - $\mathrm{Var}(\varepsilon|x) = \sigma^2$, with $\sigma \in [0, \infty)$.

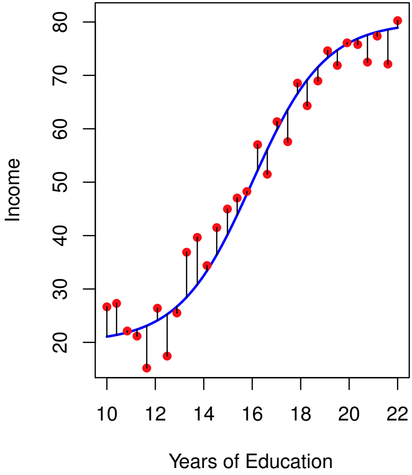
Note that we have

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

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

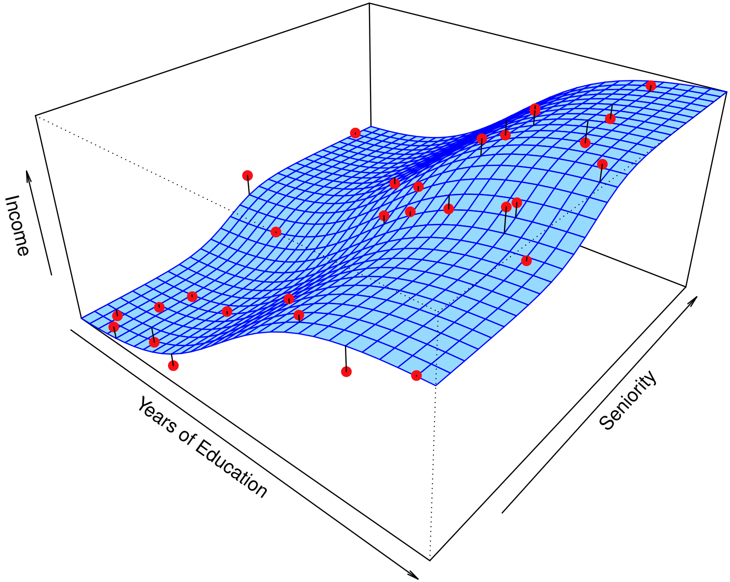
Data distribution in regression





→ Try to visualize $p_{x,y}$

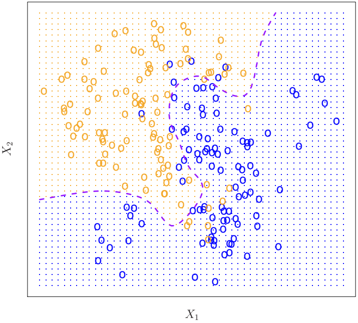
Data distribution in regression

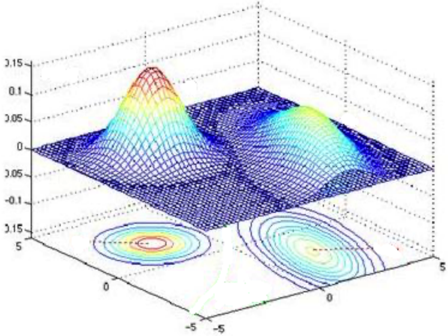


Data distribution in classification

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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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:

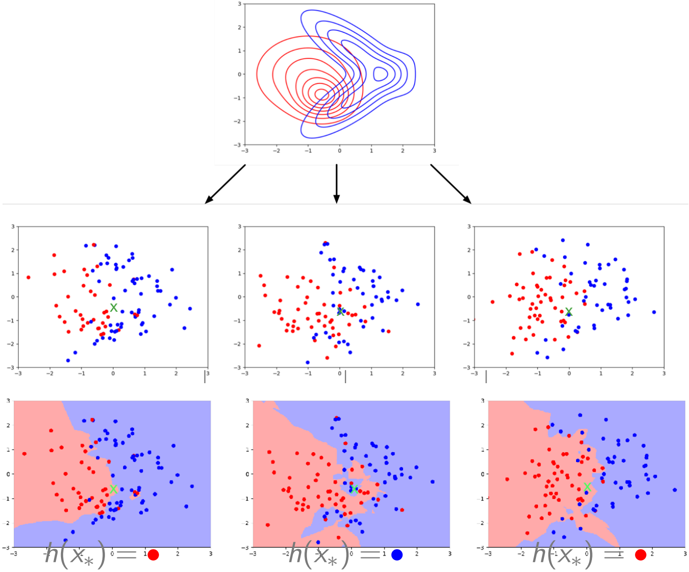
$$E_{\text{out}}(g) - E_{\text{out}}(f) = \underbrace{[E_{\text{out}}(g^*) - E_{\text{out}}(f)]}_{\text{Approximation error}} + \underbrace{[E_{\text{out}}(g) - E_{\text{out}}(g^*)]}_{\text{Estimation error}}$$

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

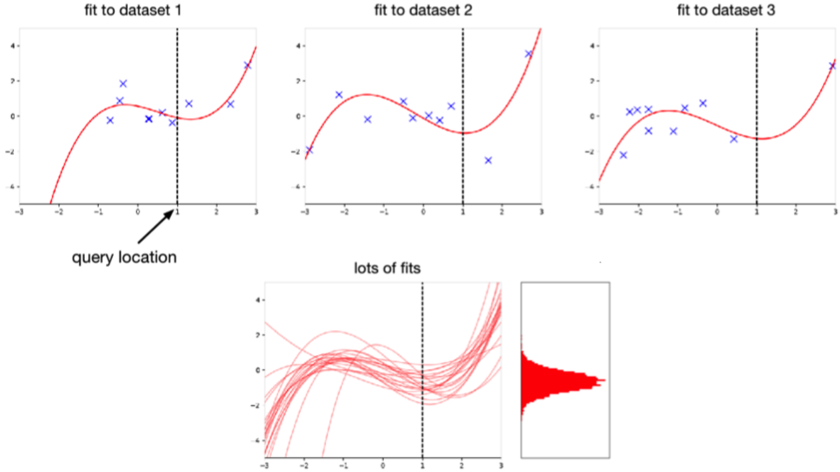
An experiment

- 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 $\mathcal{D}$.

Classification example



Regression example



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_*.

Let us expand

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

for the squared error loss $L(y, \hat{y}) = (y - \hat{y})^2$.

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The bias-variance decomposition

Recall that

$$\mathbb{E}_{y|x}[(y - g(x))^2|x] = \mathrm{Var}(y|x) + (f(x) - g(x))^2 \text{ where } f(x) = \mathbb{E}[y|x].$$

We can write

$$\begin{aligned}
&\mathbb{E}_{\mathcal{D}}\left[\mathbb{E}_{y|x}\left[(y - g(x))^2|x\right]\right] \\
&= \mathrm{Var}(y|x) + \mathbb{E}_{\mathcal{D}}[(f(x) - g(x))^2] \\
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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".

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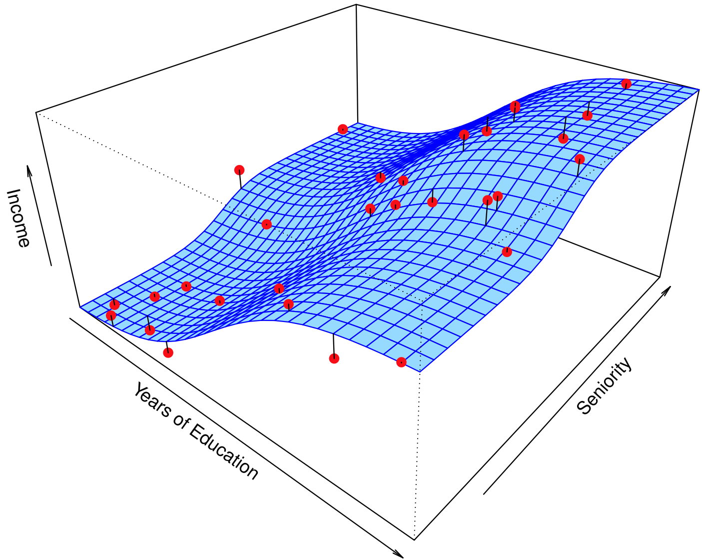
Example



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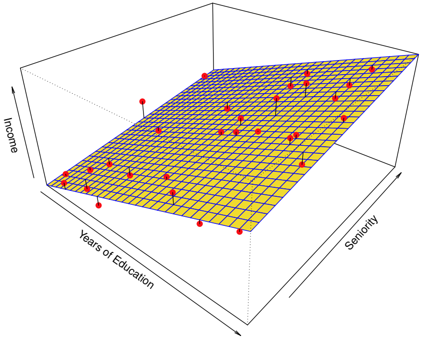
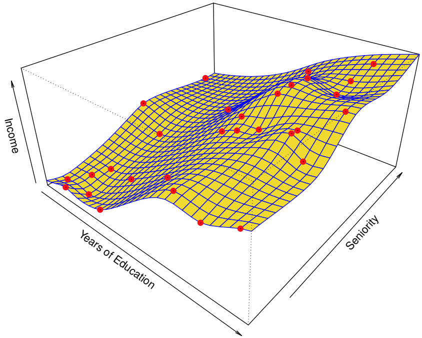

Income
Years of Education
Seniority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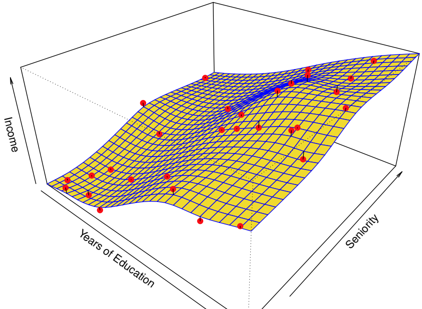
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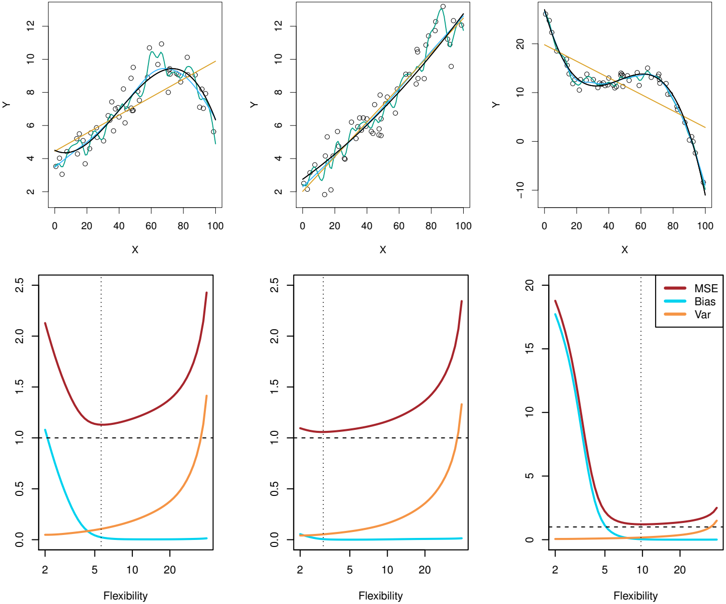
The bias-variance tradeoff



The bias-variance tradeoff

Throwing darts = predictions for each draw of a dataset