A Probabilistic Perspective

CS 4641
Machine Learning

Why probabilities?

Gives us a formal way to talk about **noise** (Frequentist)

Gives us a formal way to talk about **belief** (Bayesian)

Useful probability facts/definitions:

Notation

$$p(X) = \text{Probability of } X$$

$$0 \leq p(X) \leq 1$$

$$\int p(x)dx = 1$$

Independence

$$p(X, Y) = p(X) \cdot p(Y) \Leftrightarrow X \text{ and } Y \text{ are independent}$$

Conditional

$$p(X \mid Y) = \frac{p(X, Y)}{p(Y)}, \text{ if } p(Y) > 0$$

Bayes Rule

$$p(X \mid Y) = \frac{p(Y \mid X)p(X)}{p(Y)}$$

Expected Value

Useful facts about how **expectation** works

Definition

$$\mathbb{E}[X] = \int x \cdot p(x) dx$$

Linearity

$$\mathbb{E}[X + Y] = \mathbb{E}[X] + \mathbb{E}[Y]$$

$$\mathbb{E}[aX + b] = a\mathbb{E}[X] + b$$

Conditional

$$\mathbb{E}[X \mid Y] = \int x \cdot p(x \mid y) dx$$

Total Expectation

$$\mathbb{E}[X] = \mathbb{E}_{\mathcal{Y}}[\mathbb{E}_{\mathcal{X}}[X \mid Y]]$$

Expectation is a statistical measure of the **central tendency** of a random variable, and tells us where the "middle" of the distribution of a random variable is

Variance

Useful facts about variance

$$
\begin{aligned}
&\text{Definition} \\
&\quad \mathrm{Var}[X] = \mathbb{E}\left[(X - \mathbb{E}[X])^2\right] = \mathbb{E}[X^2] - \mathbb{E}[X]^2 \\
&\text{Constants} \\
&\mathrm{Var}[X + a] = \mathrm{Var}[X] \\
&\mathrm{Var}[aX] = a^2 \mathrm{Var}[X] \\
&\mathrm{Var}[a] = 0
\end{aligned}
$$

The variance is a statistical measure of **deviation from the mean** and gives a number for how “noisy” a random variable is.

The Bias-Variance tradeoff Proof (1)

Start with

Model, trained on S

$$\mathbb{E}_S\left[\left(y - h_\theta(\mathbf{x})\right)^2\right]$$

Arbitrary output

Arbitrary input

End with

$$(y - \mathbb{E}[h_\theta(\mathbf{x})])^2 + \mathrm{Var}[h_\theta(\mathbf{x})]$$

Where **y** is an arbitrary output, and **x** is an arbitrary input, and the expectation is taken with respect to the **distribution** of the **training data**

The Bias-Variance tradeoff Proof (2)

$$
\begin{aligned}
\mathbb{E}_S[(y - h_\theta(\mathbf{x}))^2] =& \mathbb{E}_S[(y - \mathbb{E}_S[h_\theta(\mathbf{x})] + \mathbb{E}_S[h_\theta(\mathbf{x})] - h_\theta(\mathbf{x}))^2] \\
=& \mathbb{E}_S[(y - \mathbb{E}_S[h_\theta(\mathbf{x})])^2] + \\
& \mathbb{E}_S[(\mathbb{E}_S[h_\theta(\mathbf{x})] - h_\theta(\mathbf{x}))^2] + \\
& \mathbb{E}_S[2(y - \mathbb{E}_S[h_\theta(\mathbf{x})])(\mathbb{E}_s[h_\theta(\mathbf{x})] - h_\theta(\mathbf{x}))]
\end{aligned}
$$

We **add** and **subtract** E[h(x)], then (partially) expand out the square

The Bias-Variance tradeoff Proof (3)

Let's take a closer look at the last term

$$
\begin{aligned}
\mathbb{E}_S[2(y-\mathbb{E}_S[h_\theta(\mathbf{x})])(\mathbb{E}_s[h_\theta(\mathbf{x})]-h_\theta(\mathbf{x}))] &= 2(y-\mathbb{E}_S[h_\theta(\mathbf{x})])\mathbb{E}_S[(\mathbb{E}_S[h_\theta(\mathbf{x})]-h_\theta(\mathbf{x}))] \\
&= 2(y-\mathbb{E}_S[h_\theta(\mathbf{x})])(\mathbb{E}_S[h_\theta(\mathbf{x})]-\mathbb{E}_S[h_\theta(\mathbf{x})]) \\
&= 2(y-\mathbb{E}_S[h_\theta(\mathbf{x})])(0) \\
&= 0
\end{aligned}
$$

Since **y** and E[h(x)] are **constants**, we can push the expectation inside, and the cross term vanishes!

The Bias-Variance tradeoff Proof (4)

$$\begin{aligned}
\mathbb{E}_S[(y - h_\theta(\mathbf{x}))^2] &= \mathbb{E}_S[(y - \mathbb{E}_S[h_\theta(\mathbf{x})])^2] + \mathbb{E}_S[(\mathbb{E}_S[h_\theta(\mathbf{x})] - h_\theta(\mathbf{x}))^2] \\
&= \mathbb{E}_S[(y - \mathbb{E}_S[h_\theta(\mathbf{x})])^2] + \mathrm{Var}[h_\theta(\mathbf{x})] \\
&= (y - \mathbb{E}_S[h_\theta(\mathbf{x})])^2 + \mathrm{Var}[h_\theta(\mathbf{x})] \\
&= \mathrm{Bias}(h_\theta(\mathbf{x}))^2 + \mathrm{Var}[h_\theta(\mathbf{x})]
\end{aligned}$$

So the expected loss of any hypothesis is a combination of its **bias** and its **variance**.

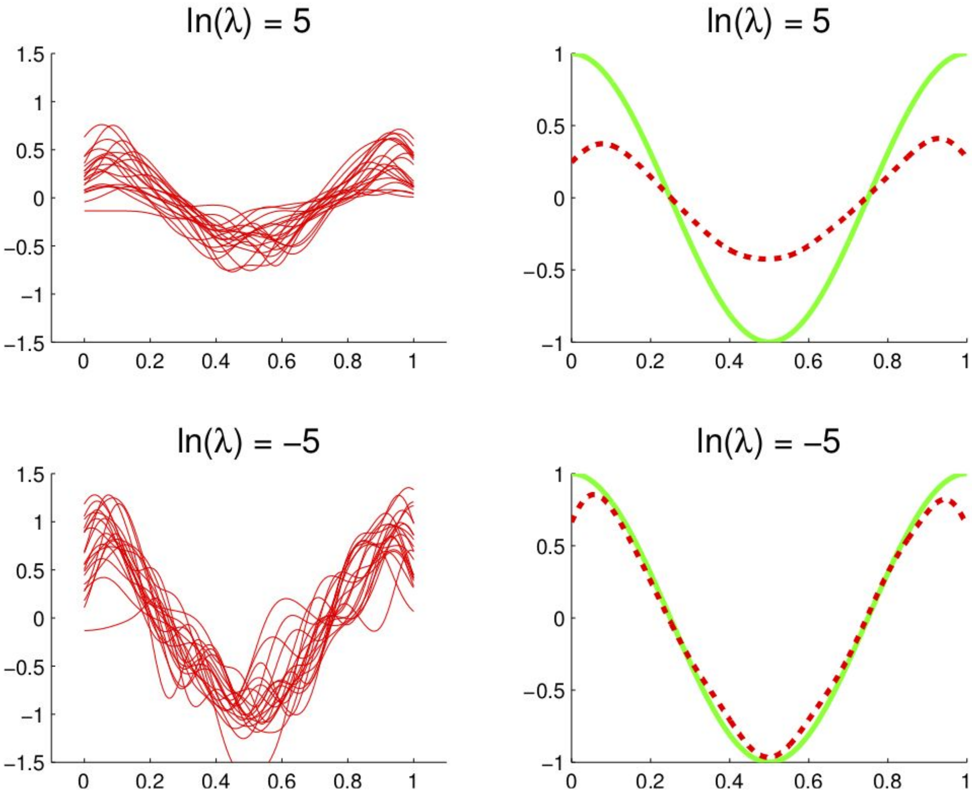
Bias is reduced by **increasing** complexity
Variance can be reduced by **decreasing** complexity

The Bias-Variance tradeoff visually

λ = regularization

High Bias
Low Variance

Low Bias
High Variance



Minimizing the Expected Loss (1)

Let’s revisit how we choose the “best” hypothesis. To start, what’s the expected loss for an arbitrary hypothesis at a given datapoint?

$$
\begin{aligned}
\mathbb{E}[(h(\mathbf{x}) - y)^2 \mid \mathbf{x}] &= \mathbb{E}\left[(h(\mathbf{x}) - \mathbb{E}[y \mid \mathbf{x}] + \mathbb{E}[y \mid \mathbf{x}] - y)^2\right] \\
&= \mathbb{E}\left[(h(\mathbf{x}) - \mathbb{E}[y \mid \mathbf{x}])^2 \mid \mathbf{x}\right] + \\
&\quad\ \mathbb{E}\left[(\mathbb{E}[y \mid \mathbf{x}] - y)^2 \mid \mathbf{x}\right] + \\
&\quad\ 2\mathbb{E}\left[(h(\mathbf{x}) - \mathbb{E}[y \mid \mathbf{x}])(\mathbb{E}[y \mid \mathbf{x}] - y) \mid \mathbf{x}\right] \\
&= \mathbb{E}\left[(h(\mathbf{x}) - \mathbb{E}[y \mid \mathbf{x}])^2 \mid \mathbf{x}\right] + \mathbb{E}\left[(\mathbb{E}[y \mid \mathbf{x}] - y)^2 \mid \mathbf{x}\right] \\
&\geq \mathbb{E}\left[(\mathbb{E}[y \mid \mathbf{x}] - y)^2 \mid \mathbf{x}\right]
\end{aligned}
$$

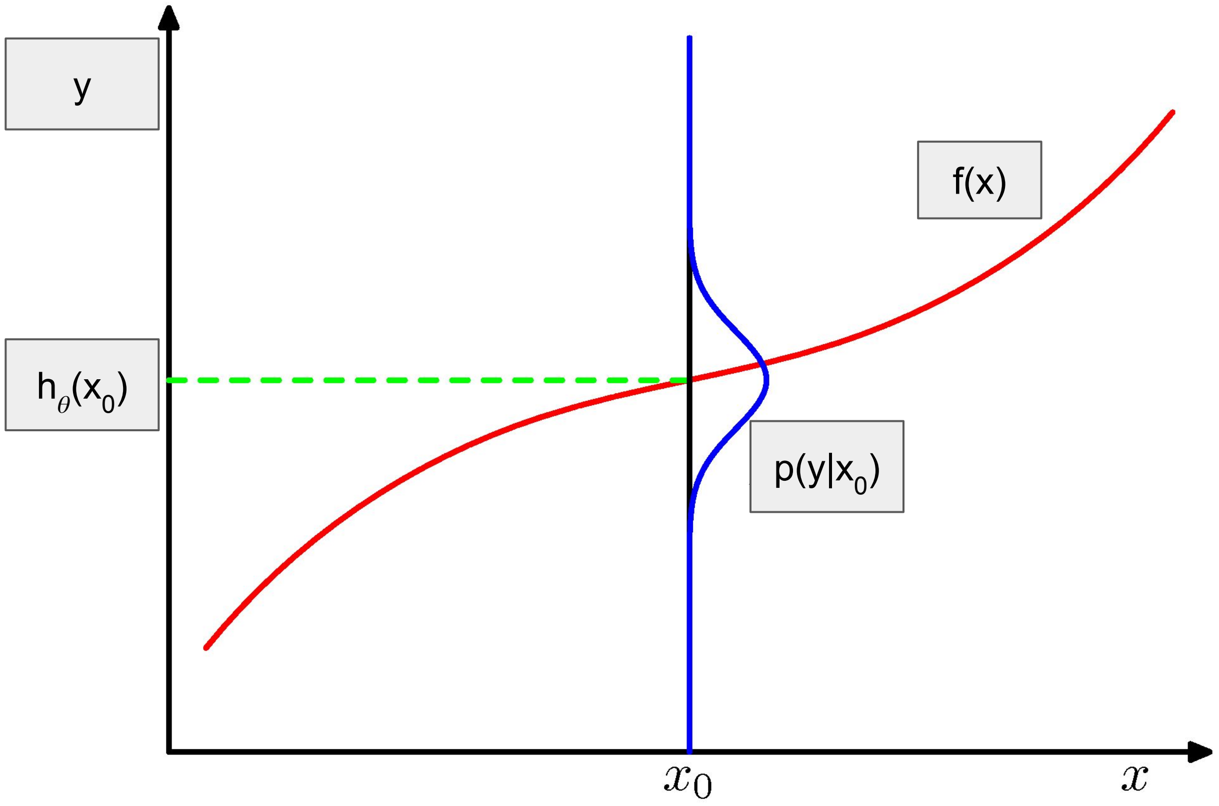
Minimizing the Expected Loss (2)

$$\mathbb{E}[(h(\mathbf{x}) - y)^2 \mid \mathbf{x}] \geq \mathbb{E}[(\mathbb{E}[y \mid \mathbf{x}] - y)^2 \mid \mathbf{x}]$$
$$\mathbb{E}[\mathbb{E}[(h(\mathbf{x}) - y)^2 \mid \mathbf{x}]] \geq \mathbb{E}[\mathbb{E}[(\mathbb{E}[y \mid \mathbf{x}] - y)^2 \mid \mathbf{x}]]$$
$$\mathbb{E}[(h(\mathbf{x}) - y)^2] \geq \mathbb{E}[(\mathbb{E}[y \mid \mathbf{x}] - y)^2]$$
$$\mathbb{E}[\mathcal{L}_S(h)] \geq \mathbb{E}[\mathcal{L}_S(\mathbb{E}[y \mid \mathbf{x}])]$$

No hypothesis can do better than predicting the expected value of y given x!

This makes sense if we think of the **noise** in the training data as being a small additive error

Conditional Expectation - Graphical View



Modeling Noise Probabilistically

Let's assume there is a "ground truth" deterministic function which generates our data, and that the samples in our dataset **S** have some small noise.

$$y^{(i)} = f(\mathbf{x}^{(i)}) + \epsilon^{(i)}$$

$$\epsilon^{(i)} \sim \mathcal{N}(0, \sigma^2)$$

$$p\left((\mathbf{x}^{(i)}, y^{(i)}) \mid f\right) = \mathcal{N}(f(\mathbf{x}^{(i)}), \sigma^2)$$

For a model parameterized by θ, we can talk about the **likelihood** that a fixed set of data was generated by that model.

$$\begin{aligned} L(h_\theta; S) &= p(S \mid h_\theta) \\ &= p((\mathbf{x}^{(1)}, y^{(1)}), (\mathbf{x}^{(2)}, y^{(2)}), \ldots, (\mathbf{x}^{(N)}, y^{(N)}) \mid h_\theta) \end{aligned}$$

Maximum Likelihood Estimation (1)

If we assume the training data is drawn I.I.D (**independent** and **identically distributed**), we can factor the likelihood

$$L(h_\theta; S) = \prod_{i=1}^{N} p((\mathbf{x}^{(i)}, y^{(i)}) \mid h_\theta)$$

Which h maximizes the likelihood?

$$\begin{aligned} \arg\max_{h \in \mathcal{H}} L(h_\theta; S) &= \arg\max_{h \in \mathcal{H}} \log L(h_\theta; S) \\ &= \arg\min_{h \in \mathcal{H}} (-\log L(h_\theta; S)) \end{aligned}$$

Maximizing the likelihood is the same thing as **minimizing** the **negative log-likelihood** (NLL)

Maximum Likelihood Estimation (2)

Putting it together in the case of Gaussian noise

$$
\begin{aligned}
\arg\max_{h \in \mathcal{H}} L(h_\theta; S) &= \arg\min_{h \in \mathcal{H}} -\log \prod_{i=1}^{N} p((\mathbf{x}^{(i)}, y^{(i)}) \mid h_\theta) \\
&= \arg\min_{h \in \mathcal{H}} -\log \prod_{i=1}^{N} \exp\left\{ \frac{-(y^{(i)} - h_\theta(\mathbf{x}^{(i)}))^2}{2\sigma^2} \right\} \\
&= \arg\min_{h \in \mathcal{H}} -\sum_{i=1}^{N} \frac{-(y^{(i)} - h_\theta(\mathbf{x}^{(i)}))^2}{2\sigma^2} \\
&= \arg\min_{h \in \mathcal{H}} \sum_{i=1}^{N} (y^{(i)} - h_\theta(\mathbf{x}^{(i)}))^2
\end{aligned}
$$

Maximum Likelihood Estimation

The MLE estimate **also** minimizes the sum of squared errors!

$$\arg\max_{h \in \mathcal{H}} L(h_\theta; S) = \arg\min_{h \in \mathcal{H}} \sum_{i=1}^{N} (y^{(i)} - h_\theta(\mathbf{x}^{(i)}))^2$$

Notes:

- We made no assumption about the hypothesis class, just the distribution of errors (zero mean normal)
- Minimizing the sum of squared errors is **equivalent** to assuming that the data has Gaussian distributed noise

Summary and preview

Wrapping up

- Probabilities let us formalize our assumptions about noise and loss functions
- The Bias-Variance tradeoff shows us how complexity, bias, and variance are related
- Regression can be thought of as estimating the conditional expectation
- Maximum Likelihood Estimation under the assumption of Gaussian noise and IID data is equivalent to minimizing the sum of squared errors

Next time

- Moving from Regression to Classification