Philosophical Fundamentals of Machine Learning

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Week 2

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Supervised Learning

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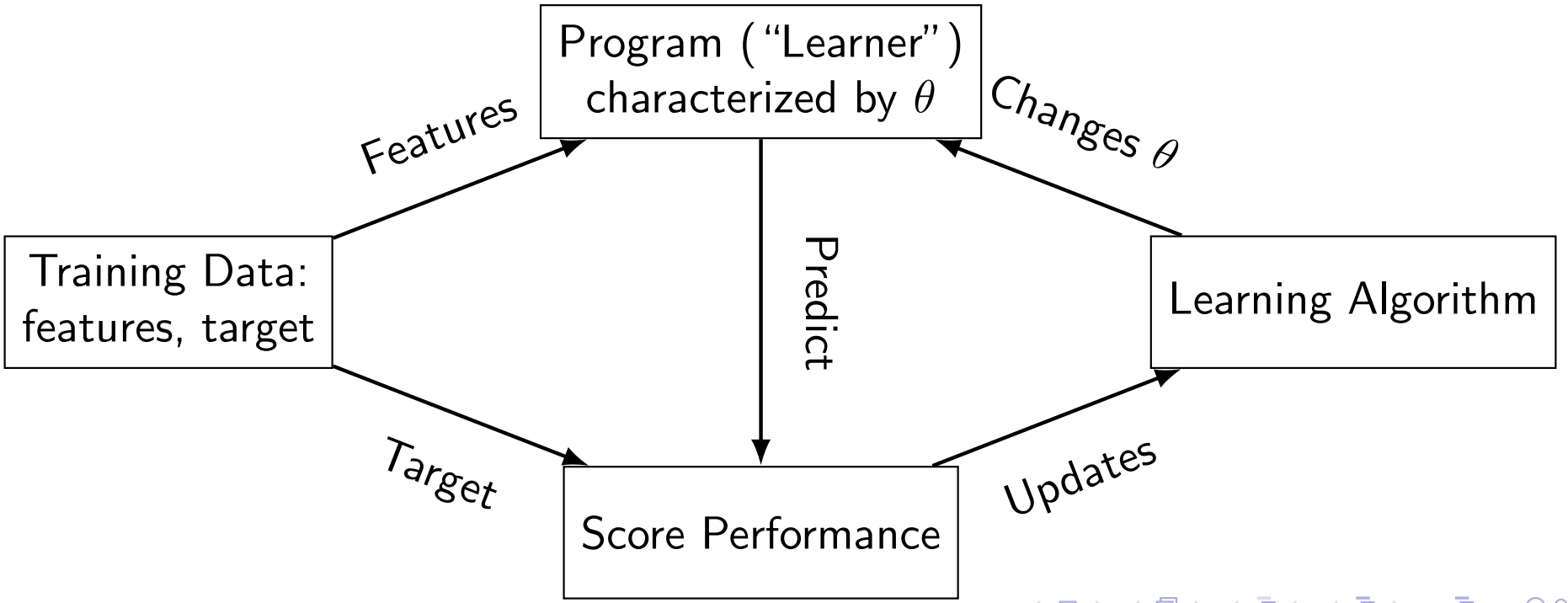

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4. Deploy and apply ML model.

The Supervised Learning Pipeline

So how do we evaluate ML models?

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The two methods we consider in this course are **Bayesian Statistical Decision Theory** and **Empirical Risk Minimization**.

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Expected Utility Theory

Example

Suppose we want to predict from some features whether a patient has cancer or not. We know that our ML model's prediction will be used to administer a drug, and we know that the drug has adverse side-effects, which can be measured by quality-adjusted life years (QALYs):

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We can think of the QALYs as measuring the relative *utility* of our predictions. If we take our goal to minimize the relative lost utility compared to how well we could do, then we have what is called a *loss* or *cost* function. **Our goal is to minimize this loss**.

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If we let our disutility be characterized by the loss function $l : Y \to \mathbb{R}$, then we say that *quality of our prediction* is given by the expected loss with respect to the target random variable Y from $Y \sim p(y)$, where the predictions of our model characterized by $\hat{y}$:

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The goal then is to find the **optimal predictor** that minimizes the expected risk:

$$\pi^*(\mathbf{x}) = \arg\min_{\hat{y} \in \hat{Y}} R(\hat{y}|\mathbf{x})$$

Example

Returning to our drug example, if we have a posterior distribution given by:

Cancer	Drugs	$l(cancer, prediction)$	$p(\cdot\|\mathbf{x})$
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$$\begin{aligned} R(c, d) &= p(c|\mathbf{x})l(c, d) + p(not\ c|\mathbf{x})l(not\ c, d) \\ &= (0.3)(5) + (0.7)(2) = 2.9 \end{aligned}$$

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The better model is then the first model.

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Example

In the previous example, our assessment of the better model would change based on how prevalent we thought cancer was. For example, if we thought $p(cancer|\mathbf{x}) = 0.1$ while $p(not\ cancer|\mathbf{x}) = 0.9$, then we would recommend the second ML model

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probability	type
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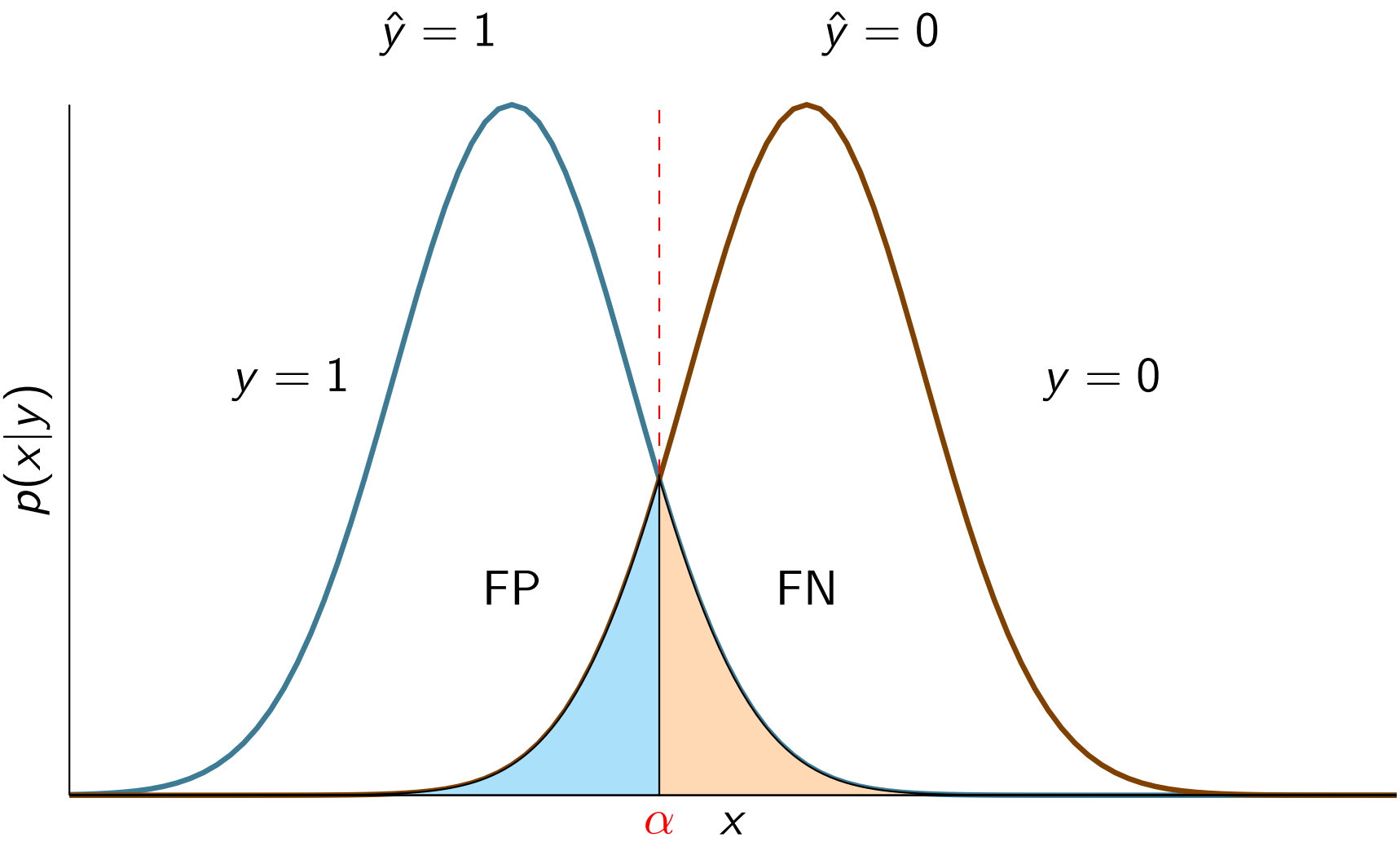
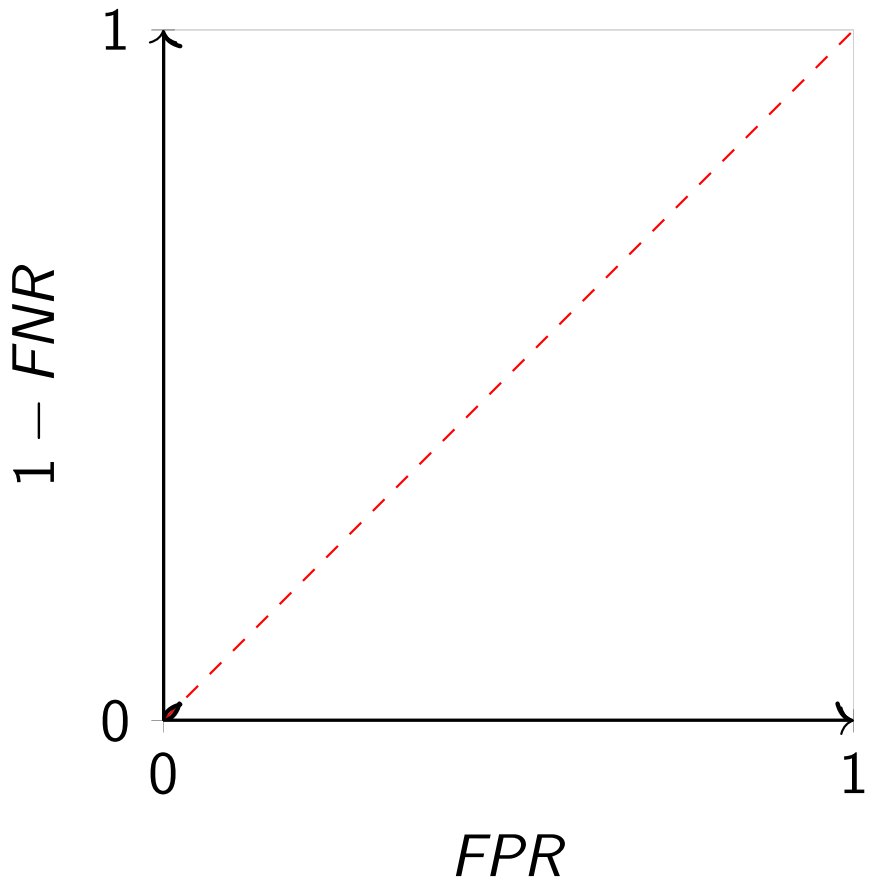
These are defined such that the TPR is $1 - FPR$ and the TNR is $1 - FPR$.

Bayesian Statistical Decision Theory



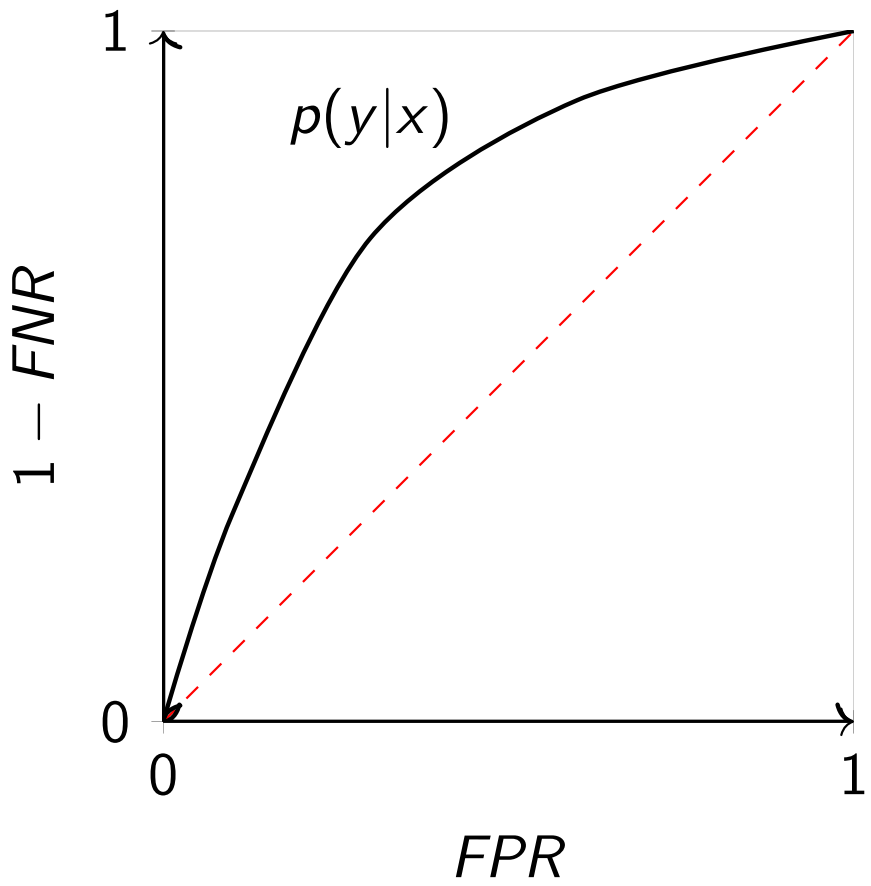
Receiver Operator Characteristic

We can plot the trade off between FPR and FNR through a **Receiver Operator Characteristic** (ROC) plot. Here the dashed red-line indicates a random guessing decision procedure.



Receiver Operator Characteristic

We can then plot the optimal Bayesian predictor in terms of our posterior probability. The area under curve (AUC) of this Bayesian predictor is as best we can do given our best beliefs. We then assess the quality of our ML algorithms by how close their AUC is to the optimal predictor:



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We turn to the second now with **Empirical Risk Minimization**.

Population Risk

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$$R(f, p^*) := \mathbb{E}_{X,Y \sim p^*(\mathbf{x},y)}[l(y, f(\mathbf{x}))] = \sum_{\mathbf{x},y \in X,Y} l(y, f(\mathbf{x}))p^*(\mathbf{x}, y)$$

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Remark

The population risk is very similar to the posterior risk in that it is a weighted average by some probability distribution and a loss function. However, they should not be confused because the population risk assumes to true, target distribution p^* that is "out in the world", and it weights the losses of our model by the *joint probability* of features and labels, instead of a posterior probability.

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Example

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1	1	1	5	0.1
1	1	0	10	
1	0	1	2	0.15
1	0	0	0	
0	1	1	5	0.05
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If we administer the drug when IBD is present, our population risk is then $(0.1)(5) + (0.15)(2) + (0.05)(10) + (0.7)(0) = 1.3$. If we do the opposite, the population risk is $(0.1)(10) + (0.15)(0) + (0.05)(5) + (0.7)(2) = 2.65$.

Empirical Risk

Remark

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$$R(f, \mathcal{D}) := \mathbb{E}_{X,Y \sim p_{\mathcal{D}}(\mathbf{x},y)}[l(y, f(\mathbf{x}))] = \frac{1}{N}\sum_{i=1}^{N} l(y^{(i)}, f(\mathbf{x}^{(i)}))$$

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IBD	Cancer	Drugs	$l(y, \hat{y})$	Counts	$p_{\mathcal{D}}(\mathbf{IBD}, Cancer)$
1	1	1	5	90	0.06
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1	0	1	2	200	0.14
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0	1	1	5	30	0.02
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Example

Suppose we collected data from a fraction of oncology practices:

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If we administer the drug when IBD is present, our empirical risk is then $(0.06)(5) + (0.14)(2) + (0.02)(10) + (0.78)(0) = 0.78$. If we do the opposite the risk is $(0.06)(10) + (0.14)(0) + (0.02)(5) + (0.78)(2) = 2.26$.

Empirical Risk Minimization

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Of course, *we don't know the population risk so we cannot calculate the generalization error directly*.

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The $\epsilon_H(N, \delta)$ is a risk bounding function parameterized by the complexity of our model

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In contrast to the internalist method of evaluation, this allows ERM to be largely about just the structure of the machine learning problem. It provides us a *reliability* assurance about how our models will perform.

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The bias-complexity tradeoff—not to be confused with the bias-variance tradeoff!

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Importantly, this error is a function of how many models we consider: if we consider more possible models, then the approximation error will go down. Letting the number of models be a measure of complexity, then **the more complex a machine learning model, the lower the approximation error**.

Bias-Complexity Tradeoff

Theorem

Suppose we want to ensure that our generalization error is less than or equal to ϵ' for all models in class $\mathcal{H}$ with probability $1 - \delta$ as we draw data $\mathcal{D}$ i.i.d. from the population distribution p^*. Then the size of our data set, N, we would need is bounded by the size $|\mathcal{H}|$:

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Remark

The number of candidate models in our set $\mathcal{H}$ is a measure of complexity of our machine learning models. This means that because we can bound our generalization error ϵ by ϵ' and supposing we ensure our dataset is the right size, then our generalization error is a function of how complex our model happens to be. **The more complex our machine learning model, the higher the generalization error**.

Bias-Complexity Tradeoff

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So when using ERM, our "what you see is what you get" guarantee forces us to choose between:

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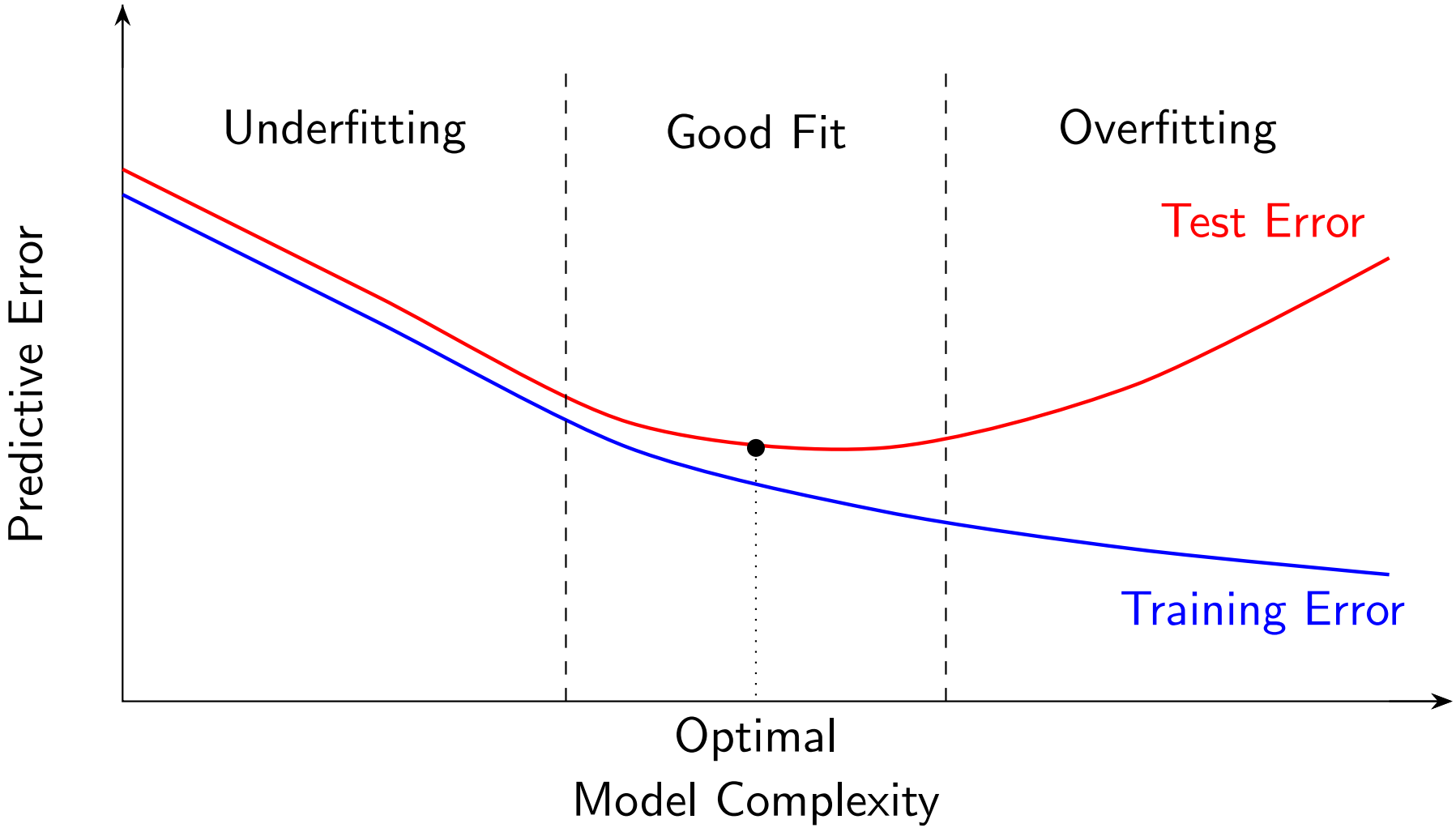
2. How well we generalize from our training data.

This is sometimes called the tradeoff between *overfitting* and *underfitting*.

Underfitting-Overfitting



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We use ERM to construct and select models during training. We check our generalization error and the degree to which we overfit or underfit the data by a **hold-out test set**. We then use AUC to measure how well we do to the optimal Bayes predictor.

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Naive Bayes

Recall

Let $A, B, C \in \Sigma$ for the probability space $(\Omega, \Sigma, \Pr)$. A and B are conditionally independent given C if $\Pr(A|B, C) = \Pr(A|C)$. Alternatively, we can define it as $\Pr(A, B|C) = \Pr(A|C)\Pr(B|C)$.

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Naive Bayes

Consider the classification problem where we suspect that features $X = \mathbf{x}$, where x_i for $i = 1, \ldots, n$ are independent of one another conditional on the class target Y, where y_k for $k = 1, \ldots, m$. That is:

$$\Pr(X = [x_1, \ldots, x_n] | Y = y_k) = \prod_{i=1}^{n} \Pr(x_i | Y = y_k)$$

We can then use this simplifying assumption to directly learn $\Pr(y|\mathbf{x})$, by using Bayes rule.

Naive Bayes continued

The Naive Bayes classifier for target $Y = y_j$:

$$\Pr(Y = y_j | X = [x_1, \ldots, x_n]) = \frac{\prod_{i=1}^{n} \Pr(x_i | Y = y_j) \Pr(Y = y_j)}{\sum_{k=1}^{m} \prod_{i=1}^{n} \Pr(x_i | Y = y_k) \Pr(Y = y_k)}$$

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Example

A common deployment of naive Bayes is as a span classifier in email: we treat the frequencies of certain words occurring, like "Nigerian Prince", as independent of one another conditional on whether the email is spam.

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k-Nearest Neighbors

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Suppose we have the classification problem with features $X = \mathbf{x}$ and class targets Y. We have some distance metric $d(\mathbf{x}, \mathbf{x}')$ between our samples, which we use to compute the K closest neighbors in our dataset $\mathcal{D}$ to a sample $\mathbf{x}$, $N_K(\mathbf{x}, \mathcal{D})$. Then our posterior predictive probability given the data is:

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Remark

When $K = 1$, we say our target is the same as that of the closest sample.

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Definition (Euclidean Distance)

A common distance metric is *Euclidean Distance*:

$$d(\mathbf{x}, \mathbf{x}') = \sqrt{(\mathbf{x} - \mathbf{x}')^\intercal (\mathbf{x} - \mathbf{x}')}$$

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Remark

We can think about K as controlling the complexity of our decision boundary between classes. Unintuitively, the lower K, the *more complex* the decision boundary while the higher the K, the *less complex* the decision boundary.

k-Nearest Neighbors