Algorithm Independent Topics

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Introduction

- Now that we've built an intuition for some pattern classifiers, let's take a step back and look at some of the more foundational underpinnings.
- Algorithm-Independent means
  - those mathematical foundations that do not depend upon the particular classifier or learning algorithm used;
  - techniques that can be used in conjunction with different learning algorithms, or provide guidance in their use.
- Specifically, we will cover
  1. Lack of inherent superiority of any one particular classifier;
  2. Some systematic ways for selecting a particular method over another for a given scenario;
  3. Methods for integrating component classifiers, including bagging, and (in depth) boosting.

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- For more information, refer to `http://www.no-free-lunch.org/`.

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  2. In these cases, most sufficiently powerful techniques (e.g., nearest neighbor methods) can perfectly learn the training set.
  3. For low-noise or low-Bayes error cases, if we use an algorithm powerful enough to learn the training set, then the upper limit of the i.i.d. error decreases as the training set size increases.
- Thus, we will use the **off-training set error**, which is the error on points not in the training set.
  - If the training set is very large, then the maximum size of the off-training set is necessarily small.

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- $P(h)$ is the prior that the algorithm will learn hypothesis h.
- $P(h|\mathcal{D})$ is the probability that the algorithm will yield hypothesis h when trained on the data $\mathcal{D}$.

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- So, what we can do is compute the expected value of the error given our dataset, which will require us to marginalize over all possible targets.

$$\mathcal{E}[E|\mathcal{D}] = \sum_{h,F} \sum_{\mathbf{x} \notin \mathcal{D}} P(\mathbf{x}) \left[1 - \delta(F(\mathbf{x}), h(\mathbf{x}))\right] P(h|\mathcal{D}) P(F|\mathcal{D}) \tag{1}$$

- We can view this as a weighted inner product between the distributions $P(h|\mathcal{D})$ and $P(F|\mathcal{D})$.
- It says that the expected error is related to
  1. all possible inputs and their respective weights $P(\mathbf{x})$;
  2. the "match" between the hypothesis h and the target F.

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- The expected off-training set error when the true function is $F(\mathbf{x})$ and the probability for the kth candidate learning algorithm is $P_k(h(\mathbf{x})|\mathcal{D})$ follows:

$$\mathcal{E}_k[E|F,n] = \sum_{\mathbf{x}\notin\mathcal{D}} P(\mathbf{x})\left[1-\delta(F(\mathbf{x}),h(\mathbf{x}))\right] P_k(h(\mathbf{x})|\mathcal{D}) \qquad (2)$$

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For any two learning algorithms $P_1(h|\mathcal{D})$ and $P_2(h|\mathcal{D})$, the following are true, independent of the sampling distribution $P(\mathbf{x})$ and the number n of training points:

1. Uniformly averaged over all target functions F,

$$\mathcal{E}_1[E|F,n] - \mathcal{E}_2[E|F,n] = 0. \tag{3}$$

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- There are no i and j such that for all $F(\mathbf{x})$, $\mathcal{E}_i[E|F,n] > \mathcal{E}_j[E|F,n]$.
- Furthermore, there is at least one target function for which random guessing is a better algorithm!

1. For any fixed training set $\mathcal{D}$, uniformly averaged over F,

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3. For any fixed training set $\mathcal{D}$, uniformly averaged over $P(F)$,

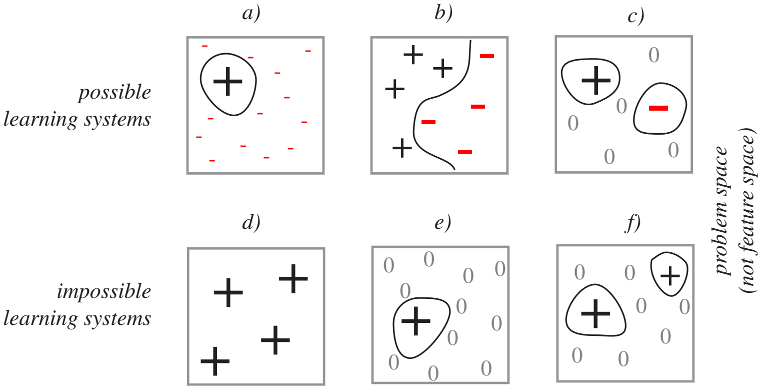
$$\mathcal{E}_1[E|\mathcal{D}] - \mathcal{E}_2[E|\mathcal{D}] = 0. \tag{6}$$

An NFLT Example

	$\mathbf{x}$	F	h_1	h_2
$\mathcal{D}$	000	1	1	1
	001	-1	-1	-1
	010	1	1	1
	011	-1	1	-1
	100	1	1	-1
	101	-1	1	-1
	110	1	1	-1
	111	1	1	-1

- Given 3 binary features.
- Expected off-training set errors are $\mathcal{E}_1 = 0.4$ and $\mathcal{E}_2 = 0.6$.
- The fact that we do not know $F(\mathbf{x})$ beforehand means that all targets are equally likely and we therefore must average over all possible ones.
- For each of the consistent 2^5 distinct target functions, there is exactly one other target function whose output is inverted for each of the patterns outside of the training set. Thus, they're behaviors are inverted and cancel.

Illustration of Part 1: A Conservation Generalization



- There is a conservation idea one can take from this: For every possible learning algorithm for binary classification the sum of performance over all possible target functions is exactly zero.

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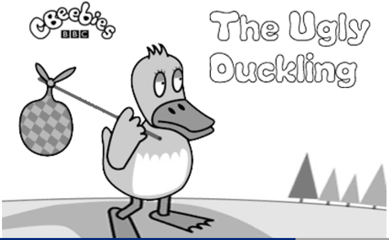
- This is a particularly important issue in practical pattern recognition scenarios when even strongly theoretically grounded methods may behave poorly.

Ugly Duckling Theorem

- Now, we turn our attention to a related question: is there any one feature or pattern representation that will yield better classification performance in the absence of assumptions?
- No! – you guessed it!



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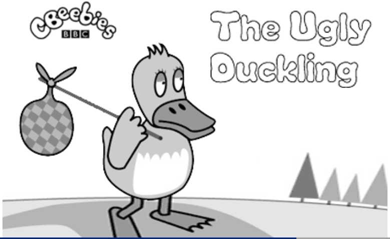

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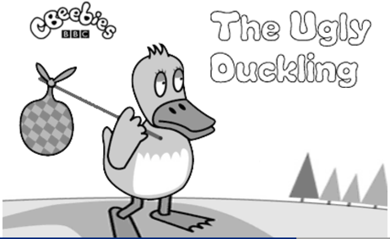
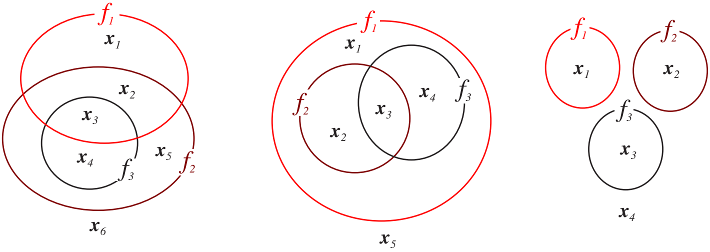
- And, of course, these assumptions may or may not be correct...



Feature Representation

- We can use logical expressions or “predicates” to describe a pattern (we will get to this later in non-metric methods).
- Denote a binary feature attribute by f_i, then a particular pattern might be described by the predicate $f_1 \wedge f_2$.
- We could also define such predicates on the data itself: $\mathbf{x}_1 \vee \mathbf{x}_2$.
- Define the **rank** of a predicate to be the number of elements it contains.



Impact of Prior Assumptions on Features

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- Suppose we have two features: f_1 represents *blind_in_right_eye*, and f_2 represents *blind_in_left_eye*. Say person $\mathbf{x}_1 = (1, 0)$ is blind in the right eye only and person $\mathbf{x}_2 = (0, 1)$ is blind only in the left eye. $\mathbf{x}_1$ and $\mathbf{x}_2$ are maximally different.

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- This is conceptually a problem: person $\mathbf{x}_1$ is more similar to a totally blind person and a normally sighted person than to person $\mathbf{x}_2$.

Multiple Feature Representations

- One can always find multiple ways of representing the same features.
- For example, we might use f'_1 and f'_2 to represent *blind_in_right_eye* and *same_in_both_eyes*, resp. Then we would have the following four types of people (in both cases):

	f_1	f_2		f'_1	f'_2
$\mathbf{x}_1$	0	0		0	1
$\mathbf{x}_2$	0	1		0	0
$\mathbf{x}_3$	1	0		1	0
$\mathbf{x}_4$	1	1		1	1

Back To Comparing Features/Patterns

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- **Key:** This result is independent of the choice of $\mathbf{x}_i$ and $\mathbf{x}_j$ (as long as they are distinct). Thus, the total number of predicates shared by two distinct patterns is constant and independent of the patterns themselves.

Ugly Duckling Theorem

- Given that we use a finite set of predicates that enables us to distinguish any two patterns under consideration, the number of predicates shared by any two such patterns is constant and independent of the choice of those patterns. Furthermore, if pattern similarity is based on the total number of predicates shared by the two patterns, then any two patterns are “equally similar.”

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- I.e., there is no problem-independent or privileged "best" set of features or feature attributes.
- The theorem forces us to acknowledge that even the apparently simply notion of similarity between patterns is fundamentally based on implicit assumptions about the problem domain.

Bias and Variance Introduction

- Bias and Variance are two measures of how well a learning algorithm matches a classification problem.
- **Bias** measures the accuracy or quality of the match: high bias is a poor match.
- **Variance** measures the precision or specificity of the match: a high variance implies a weak match.
- One can generally adjust the bias and the variance, but **they are not independent**.

Bias and Variance in Terms of Regression

- Suppose there is a true but unknown function $F(\mathbf{x})$ (having continuous valued output with noise).
- We seek to estimate $F(\cdot)$ based on n samples in set $\mathcal{D}$ (assumed to have been generated by the true $F(\mathbf{x})$).
- The regression function estimated is denoted $g(\mathbf{x}; \mathcal{D})$.
- How does this approximation depend on $\mathcal{D}$?

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- The regression function estimated is denoted $g(\mathbf{x};\mathcal{D})$.
- How does this approximation depend on $\mathcal{D}$?
- The natural measure of effectiveness is the mean square error. And, note we need to average over all training sets $\mathcal{D}$ of fixed size n:

$$\mathcal{E}_{\mathcal{D}}\left[(g(\mathbf{x};\mathcal{D}) - F(\mathbf{x}))^2\right] = \underbrace{\left(\mathcal{E}_{\mathcal{D}}\left[g(\mathbf{x};\mathcal{D}) - F(\mathbf{x})\right]\right)^2}_{\text{bias}^2} + \underbrace{\mathcal{E}_{\mathcal{D}}\left[(g(\mathbf{x};\mathcal{D}) - \mathcal{E}_{\mathcal{D}}[g(\mathbf{x};\mathcal{D})])^2\right]}_{\text{variance}} \qquad (8)$$

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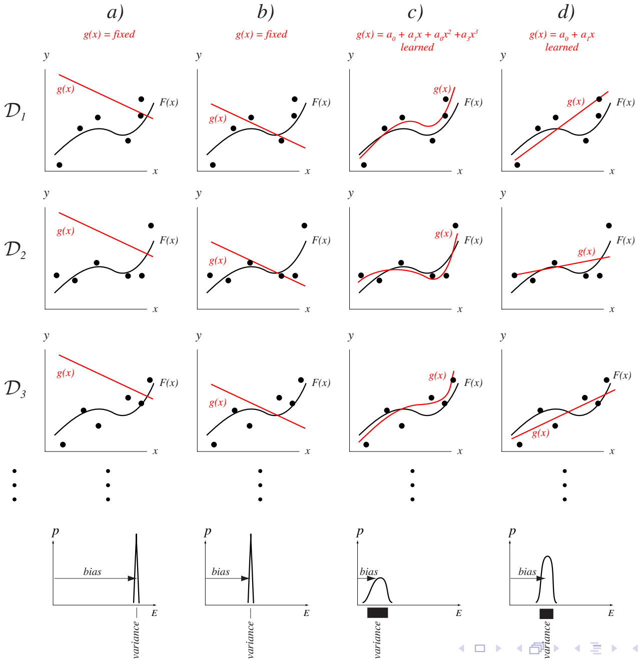
- Note, that even if an estimator is unbiased, there can nevertheless be a large mean-square error arising from a large variance term.
- The **bias-variance dilemma** describes the trade-off between the two terms above: procedures with increased flexibility to adapt to the training data tend to have lower bias but higher variance.


a)
b)
c)
d)
g(x) = fixed
g(x) = fixed
g(x) = a_0 + a_1x + a_0x^2 + a_3x^3
learned
g(x) = a_0 + a_1x
learned
$\mathcal{D}_1$
$\mathcal{D}_2$
$\mathcal{D}_3$
y
x
g(x)
F(x)
p
E
bias
variance

Bias-Variance for Classification

How can we map the regression results to classification?

- For a two-category classification problem, we can define the target function as follows

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- The target function can thus be expressed as

$$F(\mathbf{x}) = \mathcal{E}[y|\mathbf{x}] \tag{11}$$

- We want to find an estimate $g(\mathbf{x}; \mathcal{D})$ that minimizes the mean-square error:

$$\mathcal{E}_D \left[(g(\mathbf{x}; \mathcal{D}) - y)^2 \right] \tag{12}$$

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- For a given training set $\mathcal{D}$, we have the lowest error if the classifier error rate agrees with the Bayes error rate:

$$P(g(\mathbf{x}; \mathcal{D}) \neq y) = P(y_B(\mathbf{x}) \neq y) = \min[F(\mathbf{x}), 1 - F(\mathbf{x})] \tag{13}$$

- If not, then we have some increase on the Bayes error

$$P(g(\mathbf{x};\mathcal{D})) = \max[F(\mathbf{x}), 1 - F(\mathbf{x})] \tag{14}$$

$$= |2F(\mathbf{x}) - 1| + P(y_B(\mathbf{x}) = y) \ . \tag{15}$$

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- Hence, the classification error rate is linearly proportional to the **boundary error** $P(g(\mathbf{x};\mathcal{D}) \neq y_b)$, the incorrect estimation of the Bayes boundary, which is the "opposite" tail as we saw earlier in lecture 2.

$$P(g(\mathbf{x};\mathcal{D}) \neq y_B) = \begin{cases} \int_{1/2}^{\infty} p(g(\mathbf{x};\mathcal{D}))dg & \text{if } F(\mathbf{x}) < 1/2 \\ \int_{-\infty}^{1/2} p(g(\mathbf{x};\mathcal{D}))dg & \text{if } F(\mathbf{x}) \geq 1/2 \end{cases} \tag{17}$$

Bias-Variance Classification Boundary Error for Gaussian Case

- If we assume $p(g(\mathbf{x}; \mathcal{D}))$ is a Gaussian, we find

$$P(g(\mathbf{x}; \mathcal{D}) \neq y_B) =$$

$$\Phi \left[\underbrace{\mathrm{Sgn}[F(\mathbf{x}) - 1/2][\mathcal{E}_{\mathcal{D}}[g(\mathbf{x}; \mathcal{D})] - 1/2]}_{\text{boundary bias}} \underbrace{\mathrm{Var}[g(\mathbf{x}; \mathcal{D})]^{-1/2}}_{\text{variance}} \right] \tag{18}$$

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- You can visualize the boundary bias by imagining taking the spatial average of decision boundaries obtained by running the learning algorithm on all possible data sets.
- Hence, the effect of the variance term on the boundary error is highly nonlinear and depends on the value of the boundary bias.

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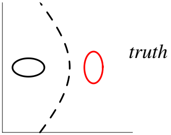
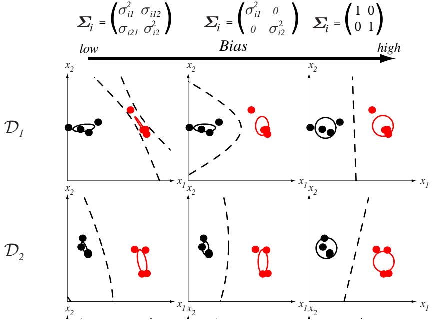
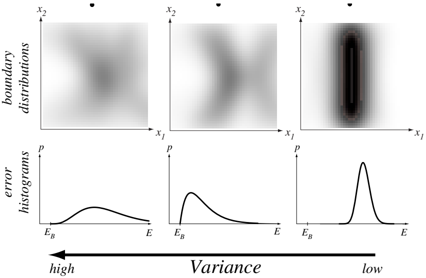
- Similarly, in classification, **variance dominates bias**.


truth


$\Sigma_i = \begin{pmatrix} \sigma_{i1}^2 & \sigma_{i12} \\ \sigma_{i21} & \sigma_{i2}^2 \end{pmatrix}$
$\Sigma_i = \begin{pmatrix} \sigma_{i1}^2 & 0 \\ 0 & \sigma_{i2}^2 \end{pmatrix}$
$\Sigma_i = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
low
Bias
high
$\mathcal{D}_1$
$\mathcal{D}_2$
x_1
x_2


boundary distributions
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p
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- **Resampling**. I.e., taking multiple datasets, perform the estimation and evaluate the boundary distributions and error histograms.
- Let's make these ideas clear in presenting two methods for resampling:
  1. Jackknife
  2. Bootstrap

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- And, the estimate of the accuracy of the mean is the sample variance, given by

$$\hat{\sigma}^2 = \frac{1}{n-1} \sum_{i=1}^{n} (x_i - \hat{\mu})^2 \tag{20}$$

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- First, define some new notation for **leave-one-out** statistic in which the statistic, such as the mean, is computed by leaving a particular datum out of the estimate. For the mean, we have

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- Next, we can define the **jackknife** estimate of the mean, that is, the mean of the leave-one-out means:

$$\mu_{(\cdot)} = \frac{1}{n}\sum_{i=1}^{n} \mu_{(i)} \tag{22}$$

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- The benefit of expressing the variance of a jackknife estimate in this way is that it generalizes to any estimator $\hat{\theta}$, such as the median. To do so, we would need to similarly compute the set of n leave-one-out statistics, $\theta_{(i)}$.

$$\text{Var}[\hat{\theta}] = \mathcal{E}\left[[\hat{\theta}(x_1, x_2, \ldots, x_n) - \mathcal{E}[\hat{\theta}]]^2\right] \tag{24}$$

$$\text{Var}_{\text{jack}}[\hat{\theta}] = \frac{n-1}{n}\sum_{i=1}^{n}(\theta_{(i)} - \theta_{(\cdot)})^2 \tag{25}$$

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- The jacknife resampling technique often gives a more satisfactory estimate of a statistic (because we can measure accuracy) than do traditional methods, but it is more computationally expensive.

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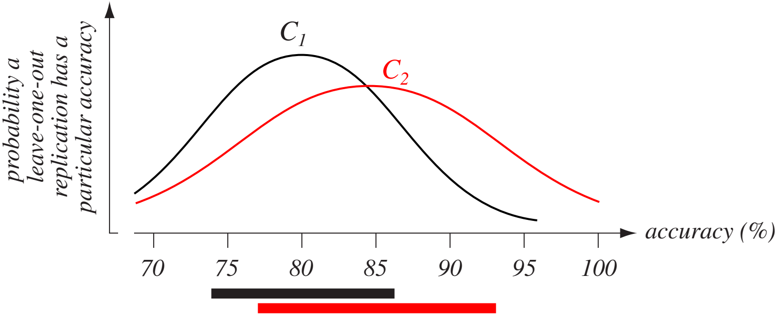
- One can apply this method to estimate the statistical significance in the comparison of two classifier designs.
- Suppose we have two trained classifiers C_1 with an accuracy of 80% and C_2 with an accuracy of 85% (both as estimated with the jackknife procedure). Is C_2 really better than C_1?

- To answer this, calculate the jackknife estimate of the variance and use traditional hypothesis testing to test statistical significance.



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- We repeat this process B times to yield B bootstrap datasets, which are treated as independent sets (although they are clearly not).
- The bootstrap estimate of a statistic θ is denoted $\hat{\theta}^{*(\cdot)}$, and, again, it is the mean of the B estimate on the individual bootstrap datasets.

$$\hat{\theta}^{*(\cdot)} = \frac{1}{B} \sum_{b=1}^{B} \hat{\theta}^{*(b)} \tag{29}$$

where $\hat{\theta}^{*(b)}$ is the estimate on bootstrap dataset b.

Bootstrap Bias Estimate

- The bootstrap estimate of the bias is

$$\text{bias}_{\text{boot}} = \frac{1}{B}\sum_{b=1}^{B}\hat{\theta}^{*(b)} - \hat{\theta} = \hat{\theta}^{*(\cdot)} - \hat{\theta} \tag{30}$$

- To increase robustness to outliers, the bootstrap method is useful for computing a **trimmed** statistic, such as the trimmed mean, in which the statistic is computed with some portion of the highest and lowest being deleted.

Bootstrap Variance Estimate

- The boostrap estimate of the variance is

$$\text{Var}_{\text{boot}}[\theta] = \frac{1}{B}\sum_{b=1}^{B}\left[\hat{\theta}^{*(b)} - \hat{\theta}^{*(\cdot)}\right]^2 \tag{31}$$

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- In general, the higher B the better the estimates of the statistic and its variance.
- A benefit of boostrap (say over jackknife) is that one can adjust B based on the available resources...

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- But, the high computational complexity of bootstrapping rarely makes this a worthwhile practice.

Cross-Validation

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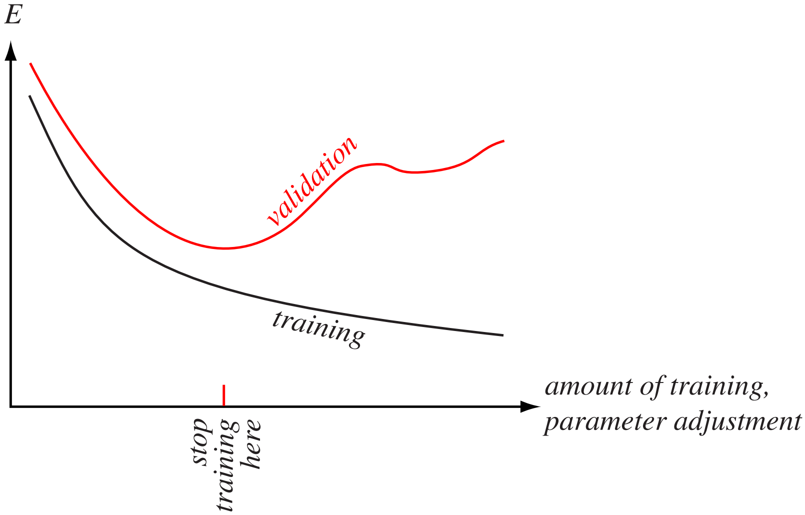
- The jackknife and bootstrap estimates of classification accuracy are closely related (or special cases of in some instances) of the method of **cross-validation**.
- **Simple Validation**
  - Split the initial dataset into two parts a training part and a **validation** part.
  - Train the classifier on the training part of the dataset.
  - But, to estimate generalization accuracy, test it on the validation part during training and halt training when we reach a minimum of this validation error.
  - It is imperative that the validation set not have points also in the training set.


E
validation
training
amount of training,
parameter adjustment
stop
training
here

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- When $m = n$.

Resampling for Classifier Design

- We just covered resampling for estimating statistics (even classification accuracies).
- Now, we want to see how resampling can help to directly improve upone classifier design.
- **Arcing**, adaptive reweighting and combing, refers to reusing or selecting data in order to improve classification.
- We will discuss two such methods
- Bagging
- Boosting (in some detail)

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- For regression, the bagged estimate is simply the average. For classification, one can count the most popular classification, or combine the classifiers in some other more sophisticated way (perhaps with yet another classifier).

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