COMS 4771 Lecture 12

1. Introduction to learning theory
2. Cross validation

Introduction to learning theory

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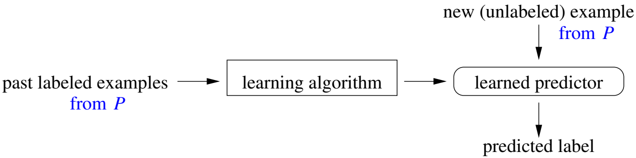

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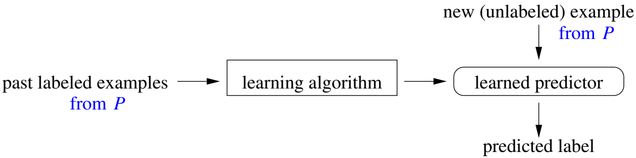

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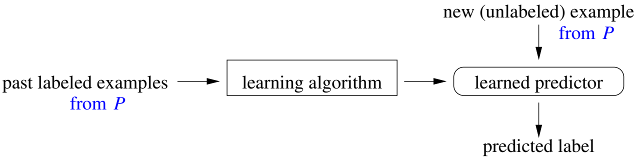

In this setting, can any learning algorithm always provide a non-trivial guarantee on the error of the predictor it returns?

No: some assumptions/conditions are required.
("No free lunch" theorem)

Assumption: realizability

Consider binary classification with $\mathcal{Y} = \{0, 1\}$.

Realizability assumption: Assume that, for a given class $\mathcal{F}$ of functions from $\mathcal{X} \to \{0, 1\}$, there exists $f^\star \in \mathcal{F}$ such that $\mathrm{err}(f^\star) = 0$.

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Examples of function classes $\mathcal{F}$:

- Rectangles in $\mathcal{X} = \mathbb{R}^2$:

$$f_{((a,b),(c,d))}(\boldsymbol{x}) = \mathbb{1}\{a \leq x_1 \leq b \text{ and } c \leq x_2 \leq d\}.$$

- Monotone conjunctions in $\mathcal{X} = \{0, 1\}^d$:

$$f_V = \mathbb{1}\{x_i = 1 \text{ for all } i \in V\}.$$

- Linear classifiers in $\mathcal{X} = \mathbb{R}^d$.

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Realizable setting is essentially the setup of **PAC Learning**, a theoretical model of learning introduced by L. Valiant (1984).

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Always possible under realizability assumption!

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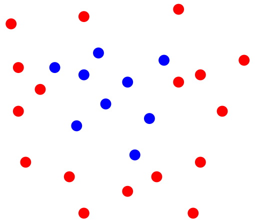
(Blue dots = positive examples.)



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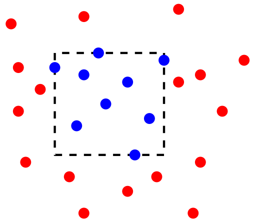

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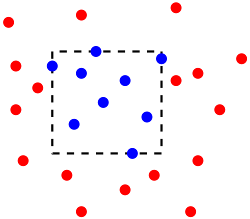

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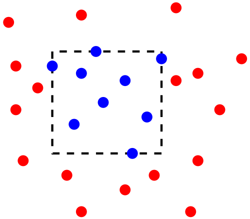

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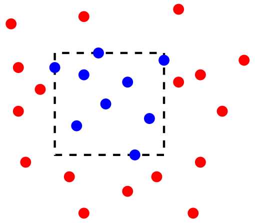

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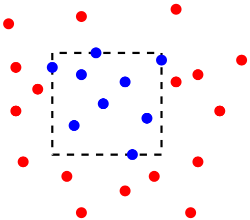

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Example: linear classifiers in $\mathbb{R}^d$ $\longrightarrow$ linear programming, Perceptron, or SVM.

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Consistent Classifier Algorithm

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for some $\varepsilon(n)$ satisfiying

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Note 2: Could also ask for

$$\mathbb{E}\left[\operatorname{err}(\hat{f})\right] \leq \varepsilon(|S|) \to 0$$

(i.e., *statistical consistency*).

Consistent Classifier Algorithm

Analysis of "Consistent Classifier Algorithm"

We know that for any $f\colon \mathcal{X} \to \{0,1\}$,

$$\Pr\left[\operatorname{err}(f) \leq \operatorname{err}(f,S) + \sqrt{\frac{2\operatorname{err}(f,S)\ln(1/\delta)}{|S|}} + \frac{2\ln(1/\delta)}{|S|}\right] \geq 1-\delta.$$

(Upper limit of confidence interval for a coin bias based on Chernoff bounds.)

error rate on sample is lower than the real error

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Generally no $\hat{f}$ is not fixed; it's chosen based on (random) training data S.

DETOUR: OVERFITTING

Consider $\mathcal{F}$ = union of up to 9 rectangles in $\mathbb{R}^2$.

Data distribution P over $\mathbb{R}^2 \times \{0, 1\}$.
(blue = positive mass)

Detour: overfitting

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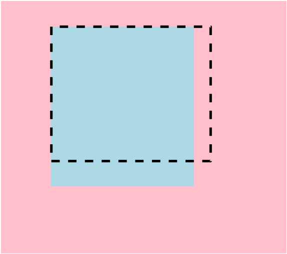

Particular rectangle function $f_1 \in \mathcal{F}$.

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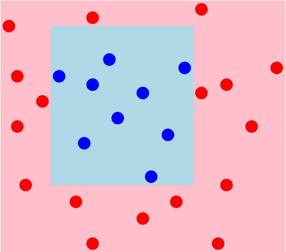

Random sample S from P.

Detour: overfitting

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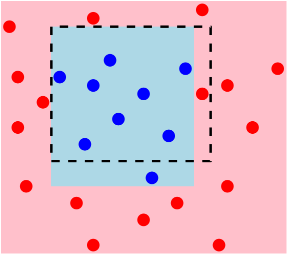

Particular rectangle function $f_1 \in \mathcal{F}$ and S.

$\mathrm{err}(f_1, S) \approx \mathrm{err}(f_1)$

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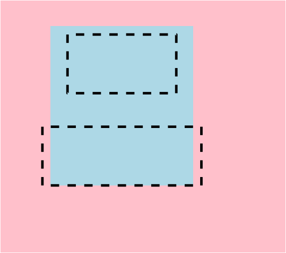

Union of rectangles function $f_2 \in \mathcal{F}$.

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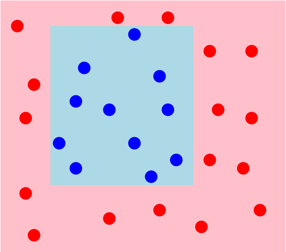
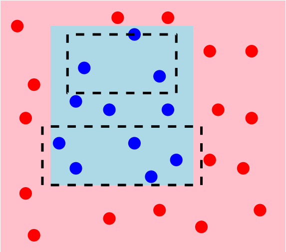


Random sample S' from P.

Consider $\mathcal{F}$ = union of up to 9 rectangles in $\mathbb{R}^2$.



Union of rectangles function $f_2 \in \mathcal{F}$ on S'.

$\mathrm{err}(f_2, S') \approx \mathrm{err}(f_2)$

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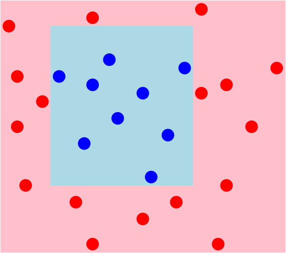
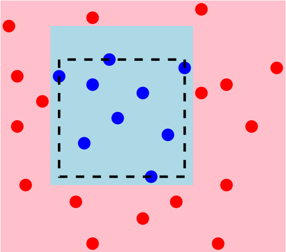
Consider $\mathcal{F} =$ union of up to 9 rectangles in $\mathbb{R}^2$.



Back to first sample S from P.

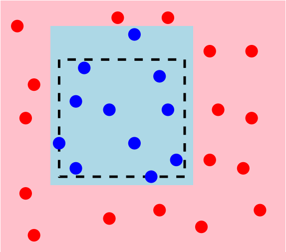
Consider $\mathcal{F}$ = union of up to 9 rectangles in $\mathbb{R}^2$.



Rectangle function $\hat{f}_{3,S} \in \mathcal{F}$ on S.

$0 = \mathrm{err}(\hat{f}_{3,S}, S) < \mathrm{err}(\hat{f}_{3,S})$

Consider $\mathcal{F}$ = union of up to 9 rectangles in $\mathbb{R}^2$.



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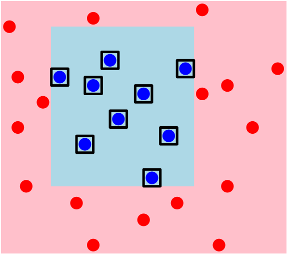

Union of rectangles $\hat{f}_{4,S} \in \mathcal{F}$ on S.

$0 = \mathrm{err}(\hat{f}_{4,S}, S) \ll \mathrm{err}(\hat{f}_{4,S})$

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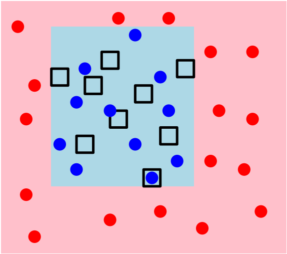

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Moral: for a classifier *chosen using the training data*, training error is not an unbiased estimate of true error.

For all $f\colon \mathcal{X} \to \{0,1\}$,

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(Upper limit of confidence interval for a coin bias based on Chernoff bounds.)

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not unbiased!

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Overkill solution: ensure upper confidence bounds hold for *all* $f \in \mathcal{F}$ *simultaneously*, with probability $\geq 1-\delta$.

Analysis of Consistent Classifier Algorithm for finite $\mathcal{F}$

Union bound: for any countable sequence of events $\mathcal{E}_1, \mathcal{E}_2, \ldots,$

$$\Pr\left[\bigcup_{i\geq 1} \mathcal{E}_i\right] \leq \sum_{i\geq 1} \Pr[\mathcal{E}_i].$$

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Apply to events $\mathcal{E}_f$ for $f \in \mathcal{F}$ given by

$$\mathcal{E}_f := \left\{\operatorname{err}(f) > \operatorname{err}(f,S) + \sqrt{\frac{2\operatorname{err}(f,S)\ln(1/\delta)}{|S|}} + \frac{2\ln(1/\delta)}{|S|}\right\}.$$

(From last slide: $\Pr[\mathcal{E}_f] \leq \delta$ for each $f \in \mathcal{F}$.)

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(From last slide: $\Pr[\mathcal{E}_f] \leq \delta$ for each $f \in \mathcal{F}$.)

Therefore, $\Pr[\bigcup_{f\in\mathcal{F}} \mathcal{E}_f] \leq |\mathcal{F}|\delta \ldots$

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intersection!!

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(From last slide: $\Pr[\mathcal{E}_f] \leq \delta$ for each $f \in \mathcal{F}$.)

Therefore, $\Pr[\bigcup_{f \in \mathcal{F}} \mathcal{E}_f] \leq |\mathcal{F}|\delta$ ... i.e., (replacing δ with $\delta/|\mathcal{F}|$)

$$\Pr\left[\forall f \in \mathcal{F} \centerdot \operatorname{err}(f) \leq \operatorname{err}(f, S) + \sqrt{\frac{2 \operatorname{err}(f, S) \ln(|\mathcal{F}|/\delta)}{|S|}} + \frac{2 \ln(|\mathcal{F}|/\delta)}{|S|}\right] \geq 1 - \delta.$$

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From last slide:

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Since the Consistent Classifier Algorithm returns $\hat{f} \in \mathcal{F}$, we know that

$$\Pr\left[\mathrm{err}(\hat{f}) \leq \mathrm{err}(\hat{f},S) + \sqrt{\frac{2\,\mathrm{err}(\hat{f},S)\ln(|\mathcal{F}|/\delta)}{|S|}} + \frac{2\ln(|\mathcal{F}|/\delta)}{|S|}\right] \geq 1-\delta.$$

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key!!!

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Consistent Classifier Algorithm for finite $\mathcal{F}$

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True error of $\hat{f}$ goes to zero as $|S| \to \infty$ at $O\left(\frac{\log(|\mathcal{F}|/\delta)}{|S|}\right)$ rate. $\square$

Generalization

Another interpretation:

- Suppose learning algorithm finds classifier $\hat{f}$ with $\mathrm{err}(\hat{f}, S) = 0$
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- Clearly only $\boxed{\text{reasonable if } \log|\mathcal{F}| \text{ is finite}}$ and not too large!

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Let $S := ((\boldsymbol{x}^{(1)}, y^{(1)}), (\boldsymbol{x}^{(2)}, y^{(2)}), \ldots, (\boldsymbol{x}^{(n)}, y^{(n)}))$. Then

$$\mathcal{F}_{|S} := \left\{ (f(\boldsymbol{x}^{(1)}), f(\boldsymbol{x}^{(2)}), \ldots, f(\boldsymbol{x}^{(n)})) : f \in \mathcal{F} \right\} \subseteq \{0,1\}^{|S|}$$

(i.e., all the different ways S can be labeled by functions in $\mathcal{F}$).

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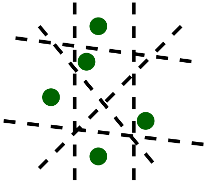

Text

(Some of the ways to label the five points by linear classifiers—there are several more.)

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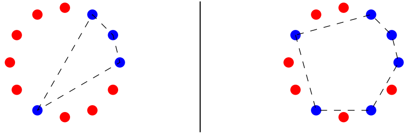
We say $\mathcal{F}$ is a **VC class**† if, as the number of training data $|S|$ increases, we are eventually in the Good situation (regardless of the actual points in S).

†VC = Vapnik-Chervonenkis (1971), same duo who proposed SVMs.

Example: arbitrary convex shapes in $\mathbb{R}^2$



For any n, there is a set of n points in $\mathbb{R}^2$ for which convex shapes realize all possible labelings. $\longrightarrow$ **Could always be in the Bad situation**.

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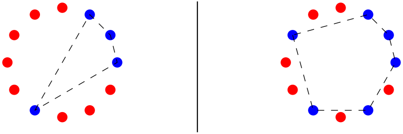

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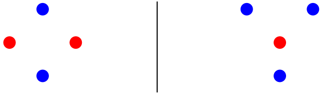

There are no sets of 4 points in $\mathbb{R}^2$ where linear classifiers realize all possible labelings. $\longrightarrow$ It turns out that $|\mathcal{F}_{|S}| \leq (c|S|)^3$.

Effective behaviors

Would be great if we could "plug-in" $|\mathcal{F}_{|S}|$ in place of $|\mathcal{F}|$ in guarantee for Consistent Classifier Algorithm:

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This straight-up "plugging-in" isn't technically legal,
but different argument implies something like $(\star)$ is true!

Recap and final remarks

- The Consistent Classifier Algorithm returns $\hat{f} \in \mathcal{F}$ with $\mathrm{err}(\hat{f}) \to 0$ as $|S| \to \infty$ with high probability, provided that:
  - labels are realized by some $f^\star \in \mathcal{F}$;
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- Guarantees depends on **complexity of function class $\mathcal{F}$** (either cardinality or effective number of behaviors).
- *Without realizability assumption,* essentially same argument applies to give a different guarantee.

  Using ERM: $\hat{f} := \arg\min_{f \in \mathcal{F}} \mathrm{err}(f, S)$, with high probability, *excess error*

get close to best classifier

$$\mathrm{err}(\hat{f}) - \min_{f \in \mathcal{F}} \mathrm{err}(f)$$

goes to zero as $|S|$ increases under same complexity conditions.

Cross validation

Objective

- Often necessary to consider many different models for a given problem (e.g., class conditional distributions in generative model classifiers, features in linear classifiers, kernel in kernelized classifiers).
- Sometimes "model" simply means particular setting of **hyper-parameters** (e.g., k in k-NN, λ in soft-margin SVM, number of nodes in decision tree).

Terminology

The problem of choosing a good model is called **model selection**.

Example: SVM with Gaussian kernel

Soft-margin SVM with Gaussian kernel

- Models indexed by regularization parameter λ and Gaussian kernel bandwidth $h > 0$:

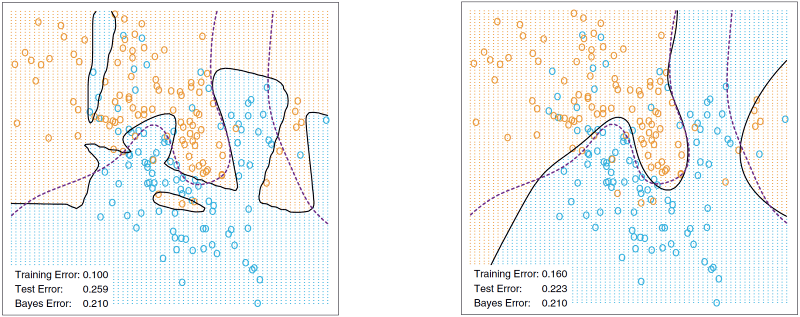
$$K(\boldsymbol{x}, \tilde{\boldsymbol{x}}) = \exp\left(-\frac{\|\boldsymbol{x} - \tilde{\boldsymbol{x}}\|_2^2}{2h}\right).$$

- Goal is to find setting of (λ, h) for which we can expect small true (generalization) error.

Naïve approach

- Also minimize over (λ, h) in SVM optimization problem.
- Leads to **overfitting**: resulting SVM classifier adapts too closely to specific properties of the training data, rather than underlying distribution.

Overfitting: illustration



- Classifier in this example has bandwidth parameter σ (similar to Gaussian kernel bandwidth).
- Small $\sigma \rightarrow$ permits curve with sharp bends
- Large $\sigma \rightarrow$ smoother curve.

(Henceforth, use $\boldsymbol{h}$ to denote particular setting of hyper-parameters / model choice.)

Hold-out validation

Model selection:

1. Randomly split data into three sets: training, validation, and test data.

Training	Validation	Test

2. Train classifier $\hat{f}_{\boldsymbol{h}}$ on Training data for different values of $\boldsymbol{h}$.
3. Compute Validation ("hold-out") error for each $\hat{f}_{\boldsymbol{h}}$: $\operatorname{err}(\hat{f}_{\boldsymbol{h}}, \text{Validation})$.
4. Selection: $\hat{\boldsymbol{h}}$ = value of $\boldsymbol{h}$ with lowest Validation error.
5. Train classifier $\hat{f}$ using $\hat{\boldsymbol{h}}$ with Training + Validation data.

Model assessment:

6. Finally: estimate the error of $\hat{f}$ using test data.

Main idea behind hold-out validation

Training	Validation	Test

Classifier $\hat{f}_h$ trained on Training data $\longrightarrow \mathrm{err}(\hat{f}_h, \text{Validation})$.

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for a lot ~
it holds

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(Making this rigorous is actually rather tricky.)

Beyond simple hold-out validation

Standard hold-out:

Training	Validation	Test

Classifier $\hat{f}_{\boldsymbol{h}}$ trained on Training data $\longrightarrow \mathrm{err}(\hat{f}_{\boldsymbol{h}}, \text{Validation})$.

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- train $\hat{f}_h$ using Validation data, and
- evaluate $\hat{f}_h$ using Training data.

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Idea: *Do both*, and average results as overall validation error for $\boldsymbol{h}$.

Model selection by K-fold cross validation

note after the classifier was selected..
we need to train on all data to get classifier

Model selection:

1. Set aside some test data.
2. Of remaining data, split into K parts ("folds") $S_1, S_2, \ldots, S_K$.
3. For each value of $\boldsymbol{h}$:
   - For each $k \in \{1, 2, \ldots, K\}$:
     - Train classifier $\hat{f}_{\boldsymbol{h},k}$ using all S_i except S_k.
     - Evaluate classifier $\hat{f}_{\boldsymbol{h},k}$ using S_k: $\mathrm{err}(\hat{f}_{\boldsymbol{h},k}, S_k)$

     Example: $K = 5$ and $k = 4$

Training	Training	Training	Validation	Training

   - Cross-validation error for $\boldsymbol{h}$: $\dfrac{1}{K}\sum_{k=1}^{K} \mathrm{err}(\hat{f}_{\boldsymbol{h},k}, S_k)$.
4. Select the value $\hat{\boldsymbol{h}}$ with lowest cross-validation error.
5. Train classifier $\hat{f}$ using selected $\hat{\boldsymbol{h}}$ with all $S_1, S_2, \ldots, S_K$.

Model assessment:

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How to choose K?

Argument for small K

Better simulates "variation" between different training samples drawn from underlying distribution.

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Training	Validation
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In practice: usually $K = 5$ or $K = 10$.

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  (Sometimes "*averaging*" the models in some way can help.)