Model Selection:

choosing the best classifier for your task

EE511 Statistical Learning

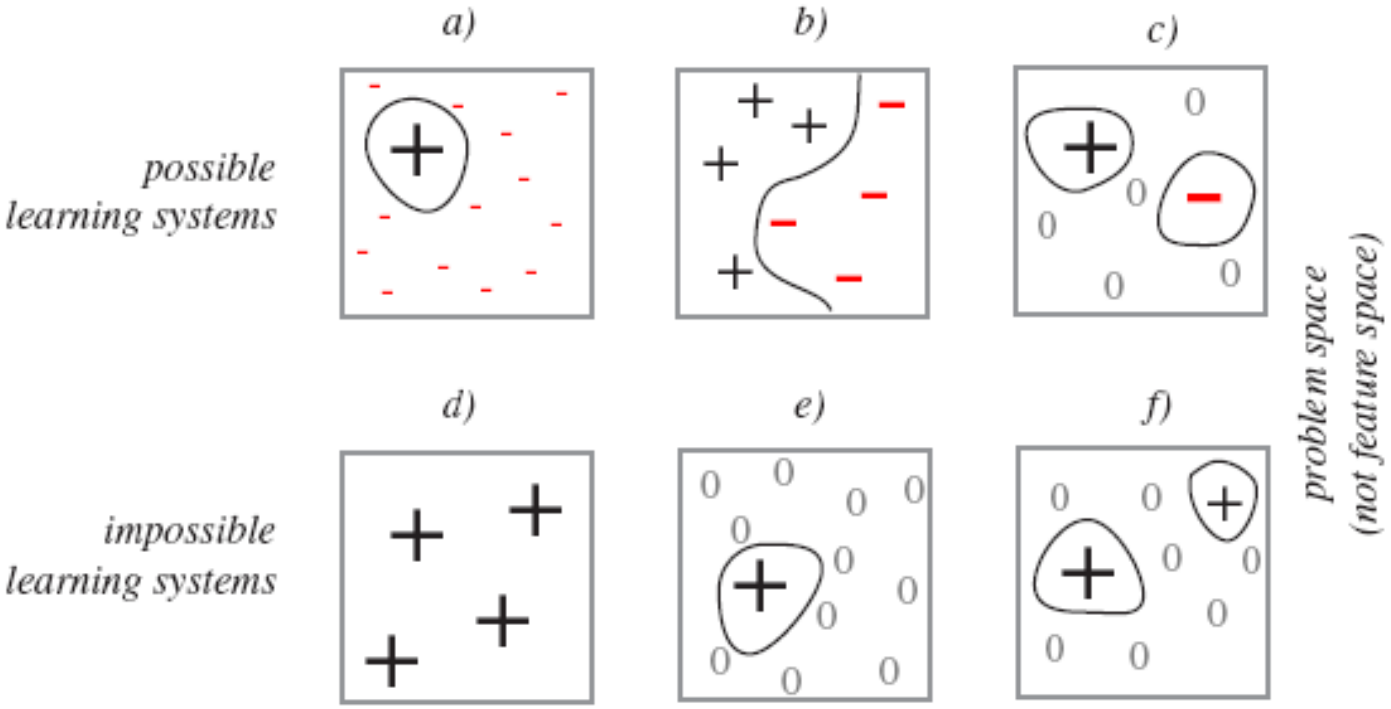
May 6, 2008

Kevin Duh

No Free Lunch Theorem

- Is there a learning algorithm that is inherently better than others?
  - Better = Lower generalization error
- "No Free Lunch Theorem" says: **NO!**
  - No algorithm is universally good for all problems.
  - Averaged over all problems, all algorithms have equal error
  - This is true independent of P(x) and data size

No Free Lunch: "Law of conservation"



- If a learning algorithm performs above-average in some problems, it will perform below-average in others (Figure from Duda, Hart, Stork, "Pattern Classification)

Model Selection

- For a particular task/dataset, an optimal algorithm may exist
- The goal of model selection:
  - Using your training data, find the model that is expected to generalize best
  - Model = different learning algorithms, different parameter settings of the same algorithm
    - Here, we'll use "classifier" and "model" interchangeably
- Related concepts:
  - Model assessment: Given a model, estimate its generalization error, error bars, etc.
  - Model averaging: Combine models as opposed to selecting the best model

Today's Agenda

1. Re-visit Bias-Variance Tradeoff
2. General concepts in Model Selection
3. Extra-sample methods
   - Cross-Validation
   - Leave-one-out error
4. Intra-sample methods
   - Bayesian model selection & BIC
   - AIC
   - MDL
5. Vapnik-Chervonekis Theory

Recurring theme:
Complexity of classifier

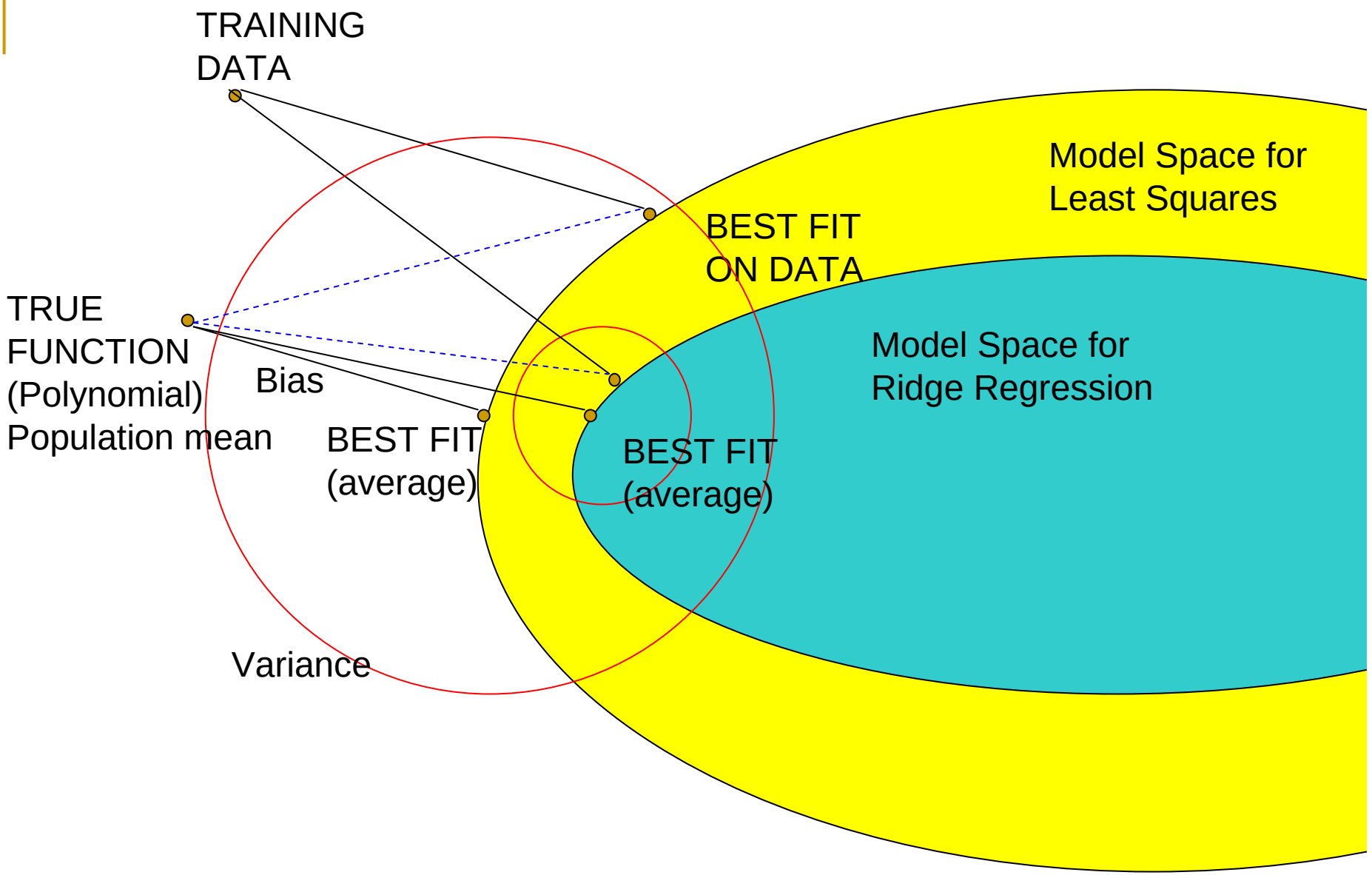
Bias-Variance Tradeoff for Regression

- Mean Squared Error = bias^2 + variance

$$E[(f(x)-y)^2] = E[f(x)-y]^2 + E[(f(x)-E[f(x)])^2]$$

  - Low bias: on average, f(x) is close to truth
  - Low variance: f(x) does not change much as training data varies

- Model selection: find the best balance
  - To reduce bias, increase model complexity (generally)
  - To reduce variance, decrease model complexity (generally)


TRAINING
DATA
Model Space for
Least Squares
BEST FIT
ON DATA
TRUE
FUNCTION
(Polynomial)
Population mean
Bias
Model Space for
Ridge Regression
BEST FIT
(average)
BEST FIT
(average)
Variance

Bias-Variance Tradeoff for Classification

- For 0-1 loss with y = {0,1}, Pr(y=1|x) = f(x):

$$\Pr(f(x) \neq y) = \Phi[\underbrace{\text{sign}(1/2 - y)E[f(x) - 1/2]}_{\text{Boundary bias}}\underbrace{\text{Var}[f(x)]^{-1/2}}_{\text{Variance}}]$$

$$\Phi[t] = 1/\sqrt{2\pi}\int_t^{\infty} e^{-u^2/2}du$$

- Different from regression case. Here:
  - Nonlinear & multiplicative interaction between bias/variance
    - If bias is negative, low variance reduces Pr(error)
    - If bias is positive, high variance reduces Pr(error)
  - Variance dominates bias
    - One reason why classifiers care so much about complexity

Today's Agenda

1. Re-visit Bias-Variance Tradeoff
2. General concepts in Model Selection
3. Extra-sample methods
   - Cross-Validation
   - Leave-one-out error
4. Intra-sample methods
   - Bayesian model selection & BIC
   - AIC
   - MDL
5. Vapnik-Chervonekis Theory

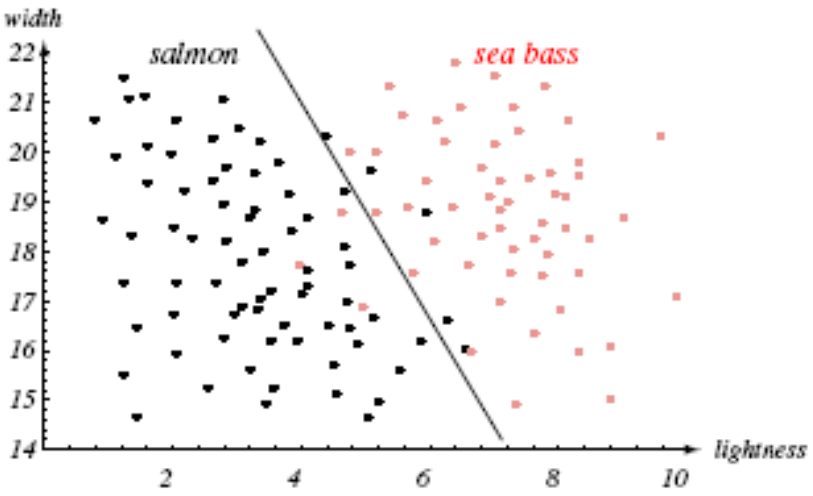
General concepts in Model Selection

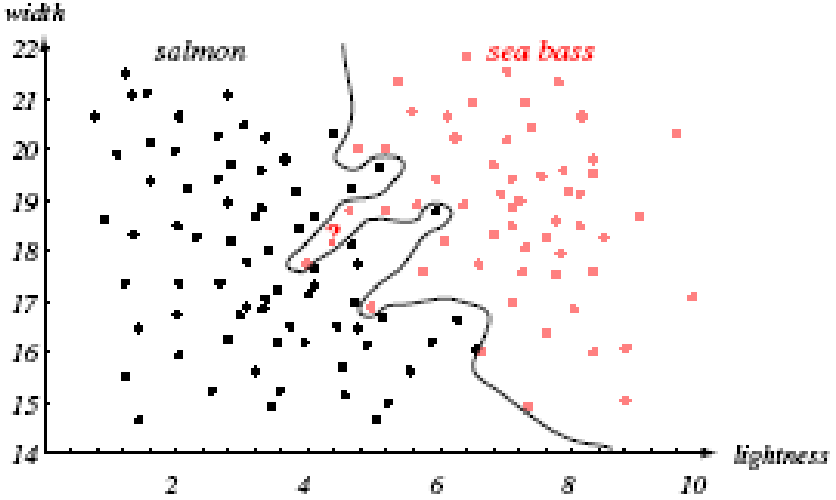
- Basic ingredients:
  - Goodness-of-fit
  - Model complexity

  } Methods vary by different definitions of these
- Training a classifier = optimizing "goodness-of-fit"
  - Objective criteria is defined
  - Learning algorithm implements an optimization procedure to pick classifier that best fits the data
    - This "selects" the best classifier among all classifiers of the same class, where "best" = attains best objective value
- **Issue: Classifiers from different classes cannot be compared using the objective**

Why can't we compare across different classes of classifiers?

- Task: binary classification
- Training objective: min error on training set
- Two different classes of classifiers: linear vs. very wiggly





- Which achieves better objective? Which will you use?

Figure from Duda, Hart, Stork, Pattern Classification

Occam's Razor

- William of Ockham (14th century logician):
  - *"entia non sunt multiplicanda praeter necessitatem"*
  - "entities should not be multiplied beyond necessity"
- In the case of statistical learning:
  - Prefer models that fit the data but have minimal complexity

Optimism of the Training Error Rate

- Goal: Low test (generalization) error

$$TestErr = E\left[L\left(Y, \hat{f}\left(X\right)\right)\right]$$

- Typically: training error rate < test error
  - Same data is used to fit the model & assess its error

$$TrainErr = \frac{1}{N}\sum_{i=1}^{n} L\left(y_i, \hat{f}\left(x_i\right)\right)$$

- Test error is a kind of extra-sample error
  - Features in the test set are not observed in the training set
  - Cross-validation methods estimate this test error using a held-out set

In-sample error

1. Assuming a data generation process: y = f(x) + noise:

$$Err_{in} = \frac{1}{N}\sum_{i=1}^{N} E_y E_{Y^{new}} L\left(Y_i^{new}, \hat{f}\left(x_i\right)\right)$$

Y^{new} = **new** response values at each of training points x_i, i=1, 2, ...,N

2. Define optimism $op \equiv Err_{in} - E_y\left(\overline{err}\right)$

For squared error, 0-1 loss functions, it can be shown: $op = \frac{2}{N}\sum_{i=1}^{N} Cov\left(\hat{y}_i, y_i\right)$
i.e. if we try too hard to fit y, then optimism is high

3. Model selection formula:
AIC, BIC, MDL, etc. can be seen as variations of this.

$$Err_{in} = E_y\left(\overline{err}\right) + \frac{2}{N}\sum_{i=1}^{N} Cov\left(\hat{y}_i, y_i\right)$$

What are properties of a good model selection method?

- Accurately estimates generalization error
  - Has low bias and variance itself
- Consistency:
  - Selects the true model (assuming it's in the class of classifiers considered) as number of training samples increases to infinity
- Computable
- No tunable parameters
- Widely applicable

Today's Agenda

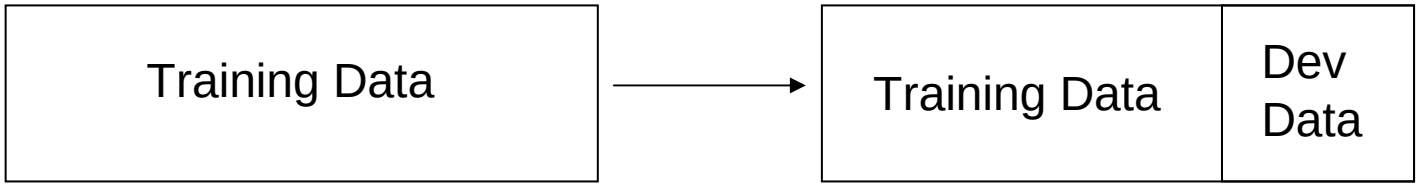
1. Re-visit Bias-Variance Tradeoff
2. General concepts in Model Selection
3. Extra-sample methods
   - Cross-Validation
   - Leave-one-out error
4. Intra-sample methods
   - Bayesian model selection & BIC
   - AIC
   - MDL
5. Vapnik-Chervonekis Theory

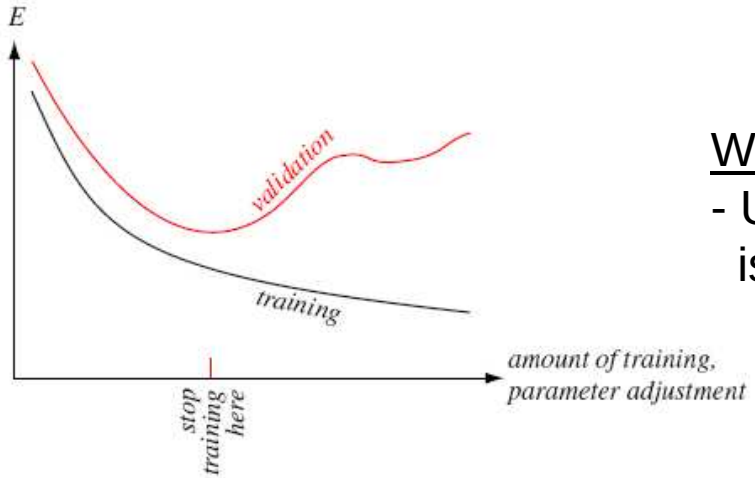
Extra-sample methods

- Directly estimate test error by using a held-out (validation) set
  - Validation, cross-validation, Leave-one-out error
  - Bootstrap
- Assumptions:
  - Validation set is similar to test set
  - Validation error is sufficiently accurate
- These methods are often used in practice
  - Usually achieves good estimates
  - Does not assume anything about the model (parametric, non-parametric) or the task (classification, regression, density estimation)

Hold-out set for model selection

- Use a development (validation) set to choose parameters/models

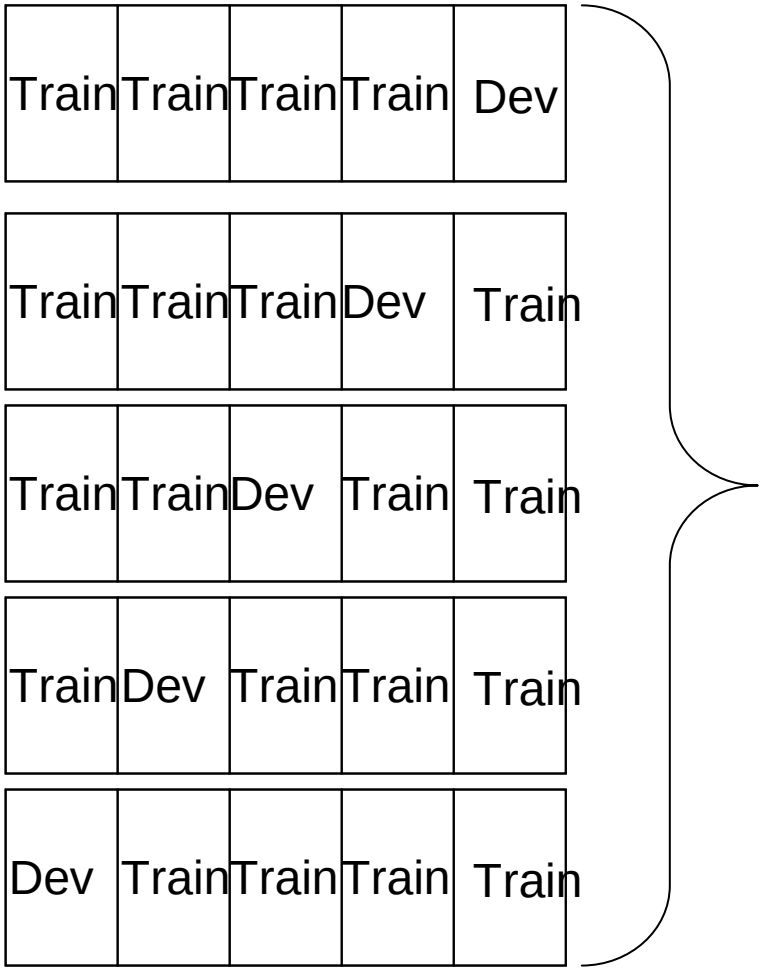




What's the proportion of dev set?

- Usually small (10-20%), since training data is needed to estimate many model parameters

K-Fold Cross-Validation



To calculate a model's performance, average the performance of each fold

-More robust than single dev set.
-Usually 5-fold or 10-fold used;
Leave-one-out error in the extreme case
-Stratified CV: maintain label proportions

How many folds in K-fold cross-validation?

Less Variance

Less Bias

LARGER K

If K=N (leave-one-out error), we get approximately unbiased estimate for test error
- but high variance due to N very similar training sets
- high computational burden (but some algorithms have clever tricks to do this)

For low K, bias may be a problem depending on size of training set

Learning Curve

If we operate at this range or above,
Cross-validation error has small bias

Large bias here
(overly pessimistic about true error)

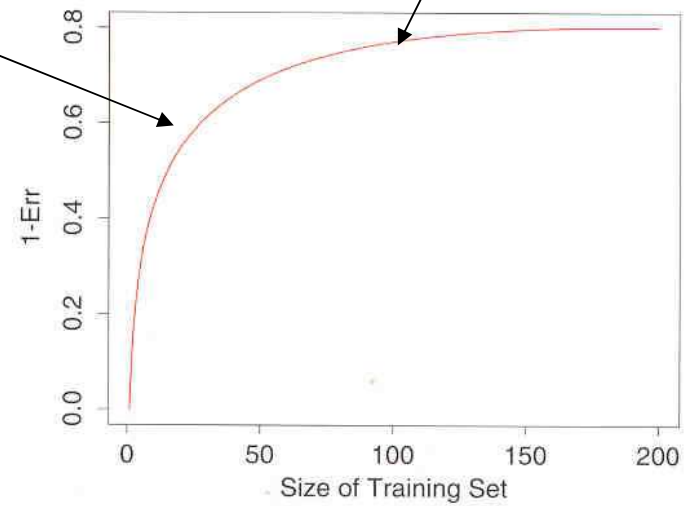


FIGURE 7.8. *Hypothetical learning curve for a classifier on a given task; a plot of* $1 - \text{Err}$ *versus the size of the training set* N*. With a dataset of* 200 *observations, fivefold cross-validation would use training sets of size* 160*, which would behave much like the full set. However, with a dataset of* 50 *observations fivefold cross-validation would use training sets of size* 40*, and this would result in a considerable overestimate of prediction error.*

- Figure from *The Elements of Statistical Learning* by Hastie, Tibshirani and Friedman.

Covariance matrix of cross-validation errors has a block structure

Corollary 1 *The covariance matrix* $\mathbf{\Sigma}$ *of cross-validation errors* $\mathbf{e} = (e_1, \ldots, e_n)'$ *has the simple block structure depicted in Figure 2: 1) all diagonal elements are identical* $\forall i$, $\mathrm{Cov}(e_i, e_i) = \mathrm{Var}[e_i] = \sigma^2$*; 2) all the off-diagonal entries of the* K $m \times m$ *diagonal blocks are identical* $\forall (i,j) \in T_k^2 : j \neq i$, $T(j) = T(i)$, $\mathrm{Cov}(e_i, e_j) = \omega$*; 3) all the remaining entries are identical* $\forall i \in T_k$, $\forall j \in T_\ell : \ell \neq k$, $\mathrm{Cov}(e_i, e_j) = \gamma$.

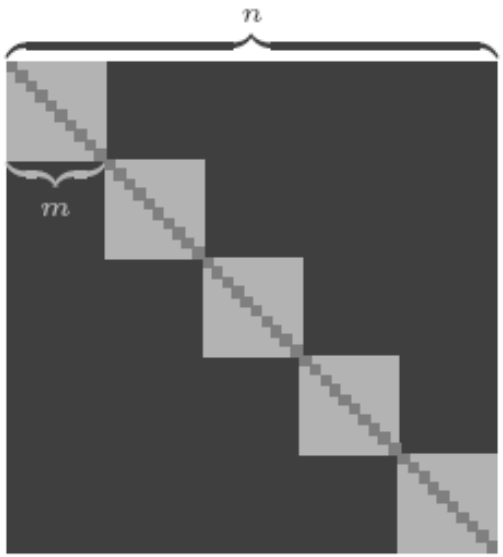


Figure 2: Structure of the covariance matrix.

From: Bengio & Grandvalet, “No unbiased estimator of variance of K-fold CV”, NIPS04

Summary of Extra-sample methods

- K-fold Cross-validation is effective in practice
  - K=5 or 10 is usually good, but do think about bias-variance questions
    - It's not a cure-all, or else it'd violate "No Free Lunch"
- Bootstrap is an alternative
  - (not discussed here)
  - Basic idea: resamples the training set with replacement to reduce variance

Today's Agenda

1. Re-visit Bias-Variance Tradeoff
2. General concepts in Model Selection
3. Extra-sample methods
   - Cross-Validation
   - Leave-one-out error
4. Intra-sample methods
   - Bayesian model selection & BIC
   - AIC
   - MDL
5. Vapnik-Chervonekis Theory

Bayesian Model Selection & BIC (1/5)

- We'll derive the BIC using Bayesian principles
- Notation:
  - D = data, w = parameters, Hi = model i
- Two levels of being Bayesian:
  - Bayesian parameter estimation

$$\mathrm{P}(w \mid D, H_i) = \frac{P(D \mid w, H_i) \cdot \mathrm{P}(w \mid H_i)}{P(D \mid H_i)}$$

Usually ignored; doesn't affect solution

    - Posterior = Likelihood x Prior / Evidence
  - Bayesian model selection

Bayesian model selection (2/5)

- Bayesian parameter estimation

$$\mathrm{P}(w \mid D, H_i) = \frac{P(D \mid w, H_i) \cdot \mathrm{P}(w \mid H_i)}{P(D \mid H_i)}$$

- Bayesian model selection

$$\mathrm{P}(H_i \mid D) = \frac{P(D \mid H_i) \cdot \mathrm{P}(H_i)}{P(D)}$$

  - Evidence P(D|Hi) is important
  - Select models H1 vs H2 based on posterior odds:

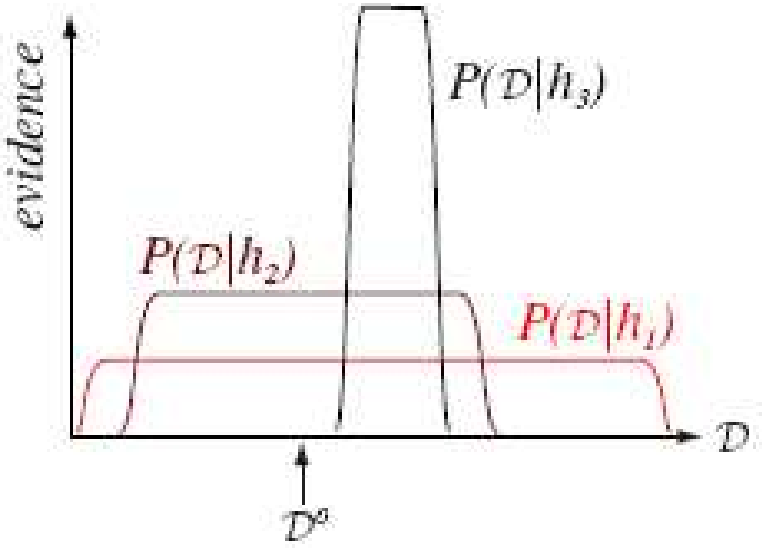
$$\frac{\mathrm{P}(H_1 \mid D)}{\mathrm{P}(H_2 \mid D)} = \frac{\mathrm{P}(H_1)}{\mathrm{P}(H_2)} \cdot \frac{\mathrm{P}(D \mid H_1)}{\mathrm{P}(D \mid H_2)}$$

Bayes Factor

Bayesian model selection (3/5)

You might imagine we need to encode the priors to penalize complex models…
But it turns out it is captured in evidence P(D|Hi) automatically

$$\frac{\mathrm{P}(H_1 \mid D)}{\mathrm{P}(H_2 \mid D)} = \frac{\mathrm{P}(H_1)}{\mathrm{P}(H_2)} \cdot \frac{\mathrm{P}(D \mid H_1)}{\mathrm{P}(D \mid H_2)}$$



Complex H will have large support because it can fit many datasets
- That implies it is less peaked

Bayesian model selection (4/5): How to evaluate the evidence?

- To compute evidence, integrate over all parameters:

$$\mathrm{P}(D \mid H_i) = \int P(D \mid w, H_i) \cdot \mathrm{P}(w \mid H_i) dw$$

- Laplacian Approximation: suppose P(w|D,Hi) is peaky at MAP solution

$$\mathrm{P}(D \mid H_i) \approx P(D \mid w_{MAP}, H_i) \cdot \mathrm{P}(w_{MAP} \mid H_i) \sigma_{w|D}$$

Width of peak

$$= P(D \mid w_{MAP}, H_i) \cdot (\frac{1}{\sigma_w} \sigma_{w|D})$$

Uniform prior over all w

Best fit likelihood Occam Factor

- Occam Factor = factor in which Hi's hypothesis space collapses after seeing data.
  - Penalizes complex models (i.e. high \sigma_w)
  - Penalizes models that fit too much to the data (i.e low \sigma_w|D)

BIC: Bayesian Information Criteria (5/5)

- BIC can be derived from a Gaussian approximation of the evidence term
  - See Raftery (1995) “Bayesian model selection in social research”, Social Methodology, Vol 25
- Basic Form:

#samples #parameters

$$BIC = -2 \cdot (\log lik) + (\log N) \cdot d.$$

  - Choose the model that has the lowest BIC
  - BIC tends to penalize complex models heavily
  - Note dependence on N

Akaike Information Criteria (AIC)

- AIC is another estimate of in-sample prediction error
  - Derived from information theoretic arguments

$$\text{For } N \to \infty: \quad -2E\left[\log \Pr_{\hat{\theta}}(Y)\right] \approx -\frac{2}{N} E\left[\log \text{lik}\right] + 2\frac{d}{N}$$

$\Pr_{\theta}(Y)$... family density for Y (containing the true density)

$\hat{\theta}$... ML estimate of θ

$$\text{loglik} = \sum_{i=1}^{N} \log \Pr_{\hat{\theta}}(y_i)$$

Maximized log-likelihood due to ML estimate of theta

AIC or BIC?

- Recall we choose model with small BIC/AIC

$$BIC = -2 \cdot (\log lik) + (\log N) \cdot d$$

$$AIC = -\frac{2}{N}(\log lik) + 2(\frac{d}{N})$$

- BIC is asymptotically consistent. AIC is not.
- AIC tends to choose more complex models as N increases
- BIC usually favors simpler models, due to strong penalty
- Asymptotically, AIC = leave-one-out; Asymptotically, BIC = cross validation with a particular K. To see this, note:

$$\log \mathrm{P}(D \mid H_i) = \log P(d_1 \mid H_i) + \log P(d_2 \mid d_1 \mid H_i) + \log P(d_N \mid d_1, d_2, \ldots d_{N-1}, H_i)$$

Cross validation examines the average of this term over reorderings of data

MDL: Minimum Description Length

- MDL can be derived from Bayesian model selection and vice versa. (But originally derived independently)
  - Replaces probability of events by code length required to communicate the event
  - L(x) = -log2(P(x)). <= length of x in bits
- MDL criteria chooses the model with the least bits.

$$MDL = -\log P(H) - \log(P(D \mid H)\delta D)$$
$$= -\log P(H \mid D) + \text{constant}$$

Model block

Data block

  - Other issues: precision of parameters

Summary of In-Sample Estimates

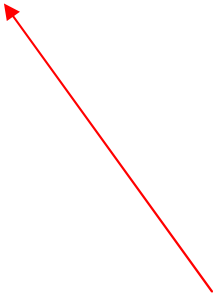
- AIC, BIC, MDL:
  - Many possible derivations
  - All contain 2 terms: goodness-of-fit & complexity
- AIC/BIC/MDL vs. Cross-Validation?
  - Personally I'd choose CV (more practical, applies to more kinds of models) unless there's good theoretical reasons to motivate AIC/BIC/MDL, etc.

Today's Agenda

1. Re-visit Bias-Variance Tradeoff
2. General concepts in Model Selection
3. Extra-sample methods
   - Cross-Validation
   - Leave-one-out error
4. Intra-sample methods
   - Bayesian model selection & BIC
   - AIC
   - MDL
5. Vapnik-Chervonekis Theory

Vapnik-Chervonenkis Theory

- VC Theory: attempts to explain learning from the statistical point of view
- Several important concepts/results
  - VC dimension & generalization error bounds
  - Structural risk minimization
  - Support vector machines



We'll mainly discuss this here in the context of model selection
but note that it is a more general theory of learning (not just model selection)

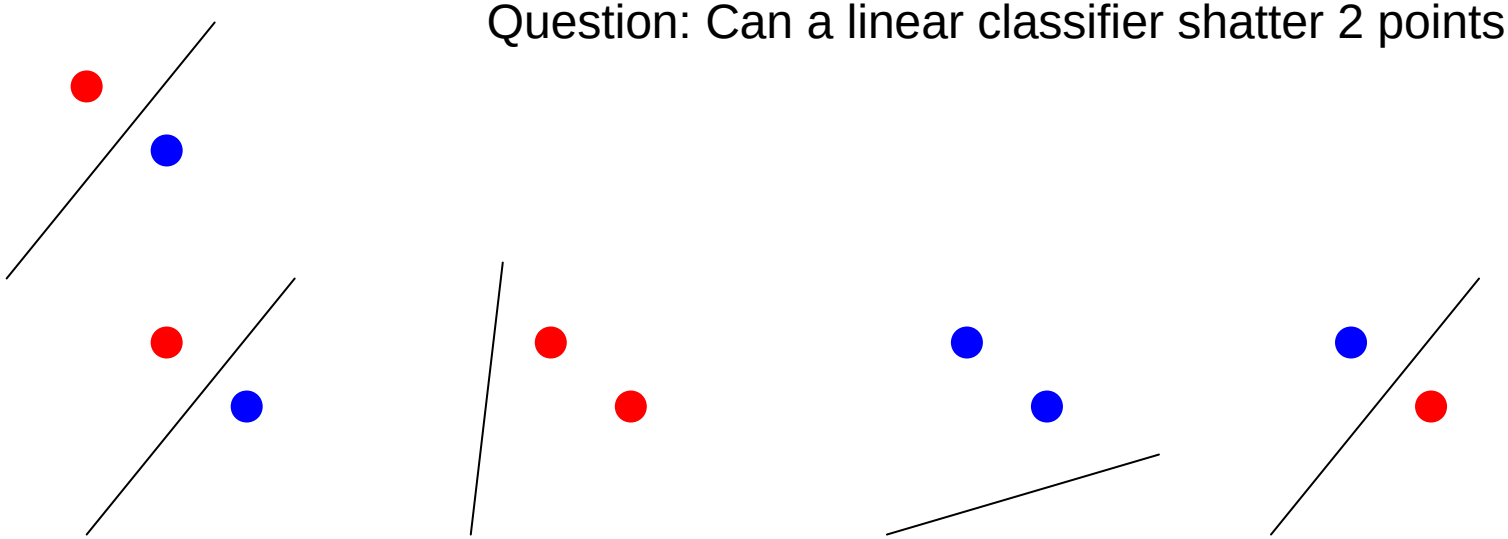
VC Dimension

- Recall that BIC/AIC/MDL counts the number of parameters in the penality term
  - For some models, #parameters is clear, but not for others (esp. non-linear models)
- VC dimension measures complexity of classifier class in relation to a general training set of m samples
  - Class of (possibly infinite) functions: {f(x,z)} is indexed by z
  - The complexity of this class is related to how many points (m) that can be shattered (i.e. 2^m labels of m points being perfectly separable)

VC Dimension Example: Shattering

- {f(x,z)} can shatter m points IFF for every possible training set of the form {(x1,y1),(x2,y2)…,(xm,ym)}, there exists some z such that f(x,z) gets zero training error

Question: Can a linear classifier shatter 2 points in 2D?



Pop Quiz

- Can a linear classifier shatter 3 points in 2D?
- Can a linear classifier shatter 4 points in 2D?

- VC Dimension = maximum number of points that can be shattered by a class of classifiers

- Whats' the VC Dimension of a linear classifier of k-dimensions?
- What function has infinite VC Dimension?

VC Dimension and Shattering (another view)

- Suppose we have a class of functions {f(x,z)} that has infinite number of elements
- But: Given m points, there are only 2^m possible sub-classes of distinct functions
- Shattering coefficient measures the number of ways a function class can separate samples
  - i.e. it's the number of different outputs (y1,y2,…ym) that can be achieved by the function class
  - If shattering coefficient = 2^m, all possible separations can be implemented, and the function class is said to be able to shatter m points
- NOTE: this means there exist a set of m patterns that can be separated in all possible ways (it does not mean all sets of m patterns need to be shattered)

VC Generalization Bound

- Vapnik showed that with probability 1-η

$$Err_{true} \le Err_{train} + \frac{\varepsilon}{2}\left(1+\sqrt{1+\frac{4 \cdot Err_{train}}{\varepsilon}}\right)$$

$$where\ \varepsilon = a_1 \frac{h\left[\log(a_2 N/h)+1\right]-\log(\eta/4)}{N}$$

$$h = VC\ \text{dimension}$$

These kind of bounds can be used for model selection, as well.
But like AIC/BIC/MDL, your mileage varies:
- some have stricter bound, some easier computable

VC Theory (Big picture)

- Main question: when does learning work?
  - Given a class of functions, we minimize training error on m points find the best f.
  - How do we know that this f leads to the lowest attainable test error as m goes to infinity (consistency)?
    - ie. f is as good as directly minimizing test error, in the limit
- Without restricting the set of functions, it turns out that empirical risk minimization is inconsistent!
  - Can you think of an example?

How to derive a VC bound

- Theorem (Vapnik & Chervonenkis): one side uniform convergence in probability,

$$\lim_{x\to\infty} P\{\sup_{f\in\mathcal{F}}(Err_{true}[f]-Err_{train}[f])>\epsilon\}=0, \forall\epsilon>0$$

  Is a necessary and sufficient condition for consistency of empirical risk minimization

- We can bound LHS as a function of VC dimension and sample size (many tricks here)

$$P\{\sup_{f\in\mathcal{F}}(Err_{true}[f]-Err_{train}[f])>\epsilon\}\le function(VC\dim, m, \epsilon)$$

- Using confidence intervals, re-express the above as:

$$Err_{true} \le Err_{train} + function(\delta, VC\dim, m, \epsilon) \text{ w/ prob } \delta$$

Overall Summary

- No Free Lunch
- Central issues:
  - How to compare models of different complexity
  - Occam's Razer
- BIC, AIC, MDL:
  - different goodness-of-fit & complexity terms
  - Bayesian model selection as motivation for BIC
- Direct estimate of test error by hold-out
  - Cross validation, Leave-one-out
- Bias-variance for classifiers, Bias-variance for estimators of test error
- VC dimension as an measure of effective classifier complexity
- VC theory: learning is all about restricting the complexity of class of classifiers (without any restriction, learning is impossible)