

Lecture 7: Model Assessment & Selection, Generalization Theory

Readings: ESL (Ch. 7), ISL (Ch. 5), Bach (Ch. 4); code

Soon Hoe Lim

September 16, 2025

Outline

- ① Part I: Practical Model Assessment & Selection
- ② Part II: Theoretical Foundations
- ③ Exercises

Overview

❗ How to understand and build models that generalize well to unseen data?

Part I: Practical Model Assessment & Selection (ESL Ch. 7, ISL Ch. 5)

Goal: Learn *how* to assess and select models in practice.

- ▶ Understanding prediction error and the bias-variance tradeoff
- ▶ Cross-validation and resampling methods
- ▶ Information criteria (AIC, BIC) for model selection
- ▶ Bootstrap methods and uncertainty quantification

Part II: Theoretical Foundations (Bach Ch. 4)

Goal: Understand *why* certain models generalize better through statistical learning theory.

- ▶ Convex surrogates for intractable problems
- ▶ Risk decomposition and the sources of error
- ▶ Rademacher complexity for generalization bounds

The Fundamental Challenge: Test vs Training Error

Definition 1: Training vs Test Error

Given training set $\mathcal{T} = \{(x_1, y_1), \dots, (x_N, y_N)\}$ and learned model \hat{f} :

- **Training Error:** $\text{err}_{\mathcal{T}} = \frac{1}{N} \sum_{i=1}^N L(y_i, \hat{f}(x_i))$

- **Test Error (Generalization Error):** $\text{Err}_{\mathcal{T}} = \mathbb{E}_{X^0, Y^0}[L(Y^0, \hat{f}(X^0)) \mid \mathcal{T}]$
where (X^0, Y^0) is a new test point independent of \mathcal{T} .

The Core Challenge: We want to minimize test error, but we can only observe training error. Low training error low test error due to **overfitting**.

► **Regression:** $L(y, \hat{f}(x)) = (y - \hat{f}(x))^2$ (squared error)

► **Classification:** $L(y, \hat{f}(x)) = \mathbb{I}[y \neq \hat{f}(x)]$ (0-1 loss)

Model Assessment vs Model Selection

Definition 2: Model Assessment vs Model Selection

- ▶ **Model Selection:** Choose the best model from a set of candidates by comparing their estimated test performance
- ▶ **Model Assessment:** Estimate the test error of our final chosen model to understand its real-world performance

⚠ **Golden Rule:** The same data should not be used for both model selection and final assessment! This leads to overly optimistic performance estimates.

In practice:

- ▶ We have **multiple candidate models** (LDA, logistic regression, SVM, etc.)
- ▶ Models have **tuning parameters** (regularization strength λ , kernel bandwidth, etc.)
- ▶ We need **reliable estimates** of how well our final model will perform

The Optimism of Training Error

Definition 3: Optimism

The **optimism** is the expected difference between test and training error: $\text{op} = \mathbb{E}_{\mathcal{T}}[\text{Err}_{\mathcal{T}}] - \mathbb{E}_{\mathcal{T}}[\text{err}_{\mathcal{T}}]$.

This gives us the fundamental relationship: $\mathbb{E}_{\mathcal{T}}[\text{Err}_{\mathcal{T}}] = \mathbb{E}_{\mathcal{T}}[\text{err}_{\mathcal{T}}] + \text{op}$

Optimism for Linear Models. For a linear model with d parameters fitted by least squares: $\text{op} = \frac{2d}{N} \sigma^2$.

💡 Each parameter "uses up" $2\sigma^2/N$ worth of degrees of freedom.

More complex models (larger d) have higher optimism:

- ▶ **Linear model:** $\text{op} \propto d$
- ▶ **Neural networks:** $\text{op} \propto \# \text{ parameters}$
- ▶ **Nonparametric methods:** $\text{op} \propto \text{effective degrees of freedom}$

Information Criteria: AIC, BIC, and C_p

These methods estimate test error by correcting the training error with a complexity penalty.

Definition 4: General Form

$$\widehat{\text{Err}} = \text{Training Error} + \text{Penalty}(\text{Model Complexity})$$

Specific Criteria

- ▶ **Mallows' C_p (for OLS regression):** $C_p = \text{err}_{\mathcal{T}} + \frac{2d}{N}\hat{\sigma}^2$ where $\hat{\sigma}^2$ is noise variance estimate (typically from full model).
- ▶ **Akaike Information Criterion (AIC):** $\text{AIC} = -2 \log \mathcal{L}(\hat{\theta}) + 2d$ For Gaussian errors, $-2 \log \mathcal{L} \propto \text{RSS}$, so $\text{AIC} \approx C_p$.
- ▶ **Bayesian Information Criterion (BIC):** $\text{BIC} = -2 \log \mathcal{L}(\hat{\theta}) + d \log N$ Since $\log N \geq 2$ for $N \geq 8$, BIC penalizes complexity more than AIC.


Information Criteria: Properties and Usage

Theoretical Properties

- ▶ **AIC:** Asymptotically equivalent to cross-validation
 - ▶ Tends to select models with complexity close to optimal for prediction
 - ▶ Can overfit in small samples
- ▶ **BIC:** Consistent model selection
 - ▶ If true model is in candidate set, BIC selects it with probability $\rightarrow 1$
 - ▶ More conservative (selects simpler models) than AIC
 - ▶ Better for interpretation, worse for prediction when truth is complex

Practical Guidelines

- ▶ **Use AIC** when primary goal is prediction accuracy
- ▶ **Use BIC** when seeking to identify "true" parsimonious model
- ▶ Both require likelihood-based models and proper parameter counting
- ▶ Not directly applicable to non-likelihood methods (SVM, trees, etc.)

 **Limitation:** Information criteria rely on asymptotic approximations and may be unreliable with small samples or misspecified models.

Cross-Validation: The Gold Standard

Cross-validation directly estimates test error by simulating the train/test process:

- ▶ Split data into training and validation sets
- ▶ Train on training set, evaluate on validation set
- ▶ Repeat with different splits to get stable estimate

K-Fold Cross-Validation

- 1: **Input:** Dataset $\mathcal{D} = \{(x_1, y_1), \dots, (x_n, y_n)\}$, number of folds K
- 2: Randomly partition \mathcal{D} into K disjoint folds: $\mathcal{D} = \mathcal{D}_1 \cup \dots \cup \mathcal{D}_K$
- 3: **for** $k = 1, 2, \dots, K$ **do**
- 4: $\mathcal{D}_{\text{train}}^{(k)} \leftarrow \mathcal{D} \setminus \mathcal{D}_k$ ▷ Training = all except fold k
- 5: $\mathcal{D}_{\text{val}}^{(k)} \leftarrow \mathcal{D}_k$ ▷ Validation = fold k
- 6: Train model: $\hat{f}^{(k)} \leftarrow \text{Learn}(\mathcal{D}_{\text{train}}^{(k)})$
- 7: Compute validation error: $\text{Err}_k \leftarrow \frac{1}{|\mathcal{D}_k|} \sum_{(x,y) \in \mathcal{D}_k} L(y, \hat{f}^{(k)}(x))$
- 8: **end for**
- 9: **Return:** $\text{CV}_K \leftarrow \frac{1}{K} \sum_{k=1}^K \text{Err}_k$

Cross-Validation: Variants and Properties

- ▶ **5-fold or 10-fold CV:** Good bias-variance tradeoff, computationally feasible. 10-fold CV most common.
- ▶ **Leave-One-Out CV (LOOCV):** $K = N$, nearly unbiased but high variance
- ▶ **Stratified CV:** Maintains class proportions in each fold (for classification)
- ▶ **Time series CV:** Respects temporal order (no future information leak)

Bias-Variance of CV Estimates

Bias:

- ▶ CV uses $(N - N/K)$ training samples vs. N for final model
- ▶ Small K (few folds) \rightarrow more bias (pessimistic estimates)
- ▶ Large K (many folds) \rightarrow less bias

Variance:

- ▶ Small $K \rightarrow$ less variance (fewer, more different estimates to average)
- ▶ Large $K \rightarrow$ more variance (many, highly correlated estimates)
- ▶ LOOCV often has very high variance

Cross-Validation for Model Selection


Model Selection via Cross-Validation

- 1: **Input:** Dataset \mathcal{D} , candidate models $\mathcal{M}_1, \dots, \mathcal{M}_m$
- 2: **for** each model \mathcal{M}_j **do**
- 3: Compute $CV_K(\mathcal{M}_j)$ using K -fold cross-validation
- 4: **end for**
- 5: $\hat{j} \leftarrow \arg \min_j CV_K(\mathcal{M}_j)$ ▷ Select best model
- 6: **Return:** Best model $\mathcal{M}_{\hat{j}}$

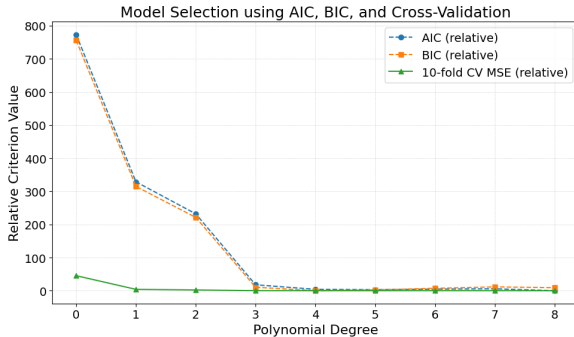
When both selecting and assessing models:

1. **Outer loop:** Split data into train/test
2. **Inner loop:** Use CV on training set to select best model
3. **Assessment:** Evaluate selected model on held-out test set

This prevents **selection bias** - overly optimistic estimates from using the same data for both selection and assessment.

 **Common Mistake:** Using the CV score from model selection as the final performance estimate. This is biased! Need separate test set or nested CV.

Example: Selecting A Polynomial Regression Model



Degree	AIC	BIC	CV_MSE
0	1335.76	1342.36	46.30
1	891.15	901.04	4.97
2	794.39	807.58	3.15
3	580.27	596.76	1.06
4	566.52	586.31	1.00
5	565.40	588.49	1.00
6	567.21	593.60	1.00
7	568.14	597.82	1.00
8	562.42	595.40	0.96

The Bootstrap

Bootstrap Principle

Idea: If we can't get new samples from the population, create "new" samples by resampling from our data.

Bootstrap Procedure

- 1: **Input:** Original dataset $\mathcal{T} = \{(x_1, y_1), \dots, (x_N, y_N)\}$
- 2: **for** $b = 1, 2, \dots, B$ **do**
- 3: Create \mathcal{T}^{*b} by sampling N points from \mathcal{T} **with replacement**
- 4: Train model: $\hat{f}^{*b} \leftarrow \text{Learn}(\mathcal{T}^{*b})$
- 5: Compute statistic of interest on \hat{f}^{*b}
- 6: **end for**
- 7: Analyze distribution of statistics across bootstrap samples

The bootstrap is another resampling method for estimating risk. It involves drawing B "bootstrap samples" of size N from the training data *with replacement*.

Each bootstrap sample omits, on average, 36.8% of the original data points. We can use these "out-of-bag" (OOB) points to form an error estimate.

Bootstrap Error Estimation

The **leave-one-out bootstrap** error estimate is:

$$\hat{R}_{boot} = \frac{1}{N} \sum_{i=1}^N \frac{1}{|C^{-i}|} \sum_{b \in C^{-i}} \ell(y_i, \hat{f}^{*b}(x_i))$$

where C^{-i} is the set of bootstrap samples that do not contain observation i .

The leave-one-out bootstrap estimate can be biased upwards because models are trained on smaller, less diverse datasets. The .632 estimators correct for this.

Definition 5: The .632 Estimator

A weighted average of the (optimistic) empirical risk and the (pessimistic) LOO bootstrap risk:

$$\hat{R}^{(.632)} = 0.368 \cdot \hat{R}_N(\hat{f}) + 0.632 \cdot \hat{R}_{boot}$$

This can fail in heavily overfit situations where $\hat{R}_N(\hat{f}) \approx 0$.

The .632+ Estimator

Definition 6: The .632+ Estimator

An improved version that adapts to the amount of overfitting.

$$\hat{R}^{(.632+)} = (1 - \hat{w}) \cdot \hat{R}_N(\hat{f}) + \hat{w} \cdot \hat{R}_{boot}$$

The weight \hat{w} adapts to the relative overfitting rate, putting more trust in the out-of-sample estimate when the model fits the training data too closely.

Bootstrap and Maximum Likelihood (see ESL Ch. 8)

Maximum Likelihood Estimation (MLE)

- ▶ MLE: $\hat{\theta} = \arg \max_{\theta} \prod_{i=1}^N f(y_i; \theta)$
- ▶ Under regularity: $\hat{\theta}$ is approximately normal with variance $\propto 1/N$
- ▶ Variance can be estimated using *Fisher information*:
$$I(\theta) = \mathbb{E} \left[-\frac{\partial^2}{\partial \theta^2} \log f(Y; \theta) \right]$$

Bootstrap Inference

- ▶ Resample data with replacement, refit model \Rightarrow distribution of $\hat{\theta}^*$
- ▶ Provides standard errors, confidence intervals, bias estimates
- ▶ Practical when analytic formulas (like Fisher info) are hard

💡 MLE gives asymptotic theory, bootstrap gives practical inference.

Method Comparison and Recommendations

Method	Pros	Cons
AIC/BIC/C_p	Fast computation, well-established theory, good for linear models	Requires likelihood or OLS, assumes model is approximately correct, can be unreliable in small samples
10-Fold CV	Widely applicable, minimal assumptions, direct test error estimate	Computationally intensive ($10\times$ cost), can be unstable with small datasets
LOOCV	Nearly unbiased for test error, deterministic result	Very high variance, extremely expensive, can be unstable
Bootstrap	More stable than LOOCV, provides uncertainty estimates, handles complex models well	More complex to implement, can still have bias issues, requires many bootstrap samples
Validation Set	Simple to understand and implement, fast	Reduces effective sample size, can be unreliable with small datasets

Practical Guidelines

1. **For most applications:** Use 10-fold cross-validation
 - ▶ Excellent bias-variance tradeoff
 - ▶ Works with any learning algorithm
 - ▶ Widely accepted and understood
2. **For linear models with likelihood:** Consider AIC/BIC as faster alternatives
 - ▶ AIC for prediction-focused applications
 - ▶ BIC for model interpretation and parsimony
3. **For very small datasets ($N < 100$):** Use LOOCV or bootstrap
 - ▶ Every sample counts
 - ▶ Higher variance acceptable given limited data
4. **For model selection + assessment:** Use nested CV or train/validation/test split
 - ▶ Prevents optimistic bias
 - ▶ Essential for honest performance reporting

From Practice to Theory

- ▶ **Part I (Practice):** Data-driven heuristics for estimating test error
 - ▶ Cross-validation, bootstrap, AIC/BIC
- ▶ **Limitation:** These methods work well in practice, but do not explain *why* models generalize.
- ▶ **Part II (Theory):** Statistical Learning Theory
 - ▶ Why does empirical risk approximate expected risk?
 - ▶ How does model complexity affect generalization?

We will only attempt to give a brief introduction to statistical learning theory here (see, e.g., Bach Ch. 4 & 7 and <https://cs.nyu.edu/~mohri/mlbook/> for full details).

The Learning Problem: Formal Setup

Definition 7: Statistical Learning Framework

- ▶ **Data:** $(x_1, y_1), \dots, (x_N, y_N)$ drawn i.i.d. from unknown distribution P on $\mathcal{X} \times \mathcal{Y}$
- ▶ **Goal:** Learn function $f : \mathcal{X} \rightarrow \mathcal{Y}$ that minimizes expected risk:

$$R(f) = \mathbb{E}_{(x,y) \sim P}[\ell(y, f(x))]$$

- ▶ **Bayes Optimal:** $f^* = \arg \min_f R(f)$ with $R^* = R(f^*)$
- ▶ **Our Focus:** Methods based on **Empirical Risk Minimization (ERM)**:

$$\hat{f} = \arg \min_{f \in \mathcal{F}} \hat{R}(f) = \arg \min_{f \in \mathcal{F}} \frac{1}{N} \sum_{i=1}^N \ell(y_i, f(x_i))$$

Key Challenge: For binary classification with 0-1 loss, this is a combinatorial optimization problem. We need better approaches!

The Convexification Strategy

For binary classification ($\mathcal{Y} = \{-1, 1\}$) with 0-1 loss:

1. Learn real-valued function $g : \mathcal{X} \rightarrow \mathbb{R}$ using convex surrogate loss $\Phi(yg(x))$
2. Make predictions via $f(x) = \text{sign}(g(x))$

Benefits:

- ▶ **Computational:** Convex optimization (global optimum, efficient algorithms)
- ▶ **Theoretical:** Enables Rademacher complexity analysis
- ▶ **Practical:** Allows gradient-based methods and principled regularization

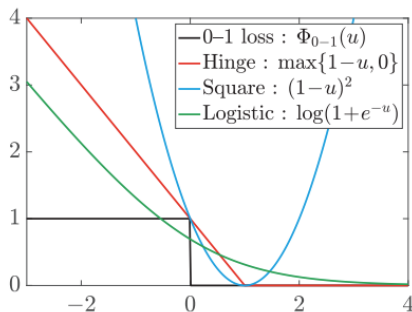
For binary classification, consider surrogate losses of the form $\Phi(yg(x))$ where $yg(x)$ is the **margin**.

- ▶ **Margin** > 0 : Correct classification with confidence
- ▶ **Margin** < 0 : Misclassification

Convexification with Calibrated Surrogate Losses

A surrogate loss Φ is **calibrated** if minimizing $\mathbb{E}[\Phi(yg(x))]$ leads to the Bayes optimal classifier. All losses below are calibrated:

- ▶ **Hinge Loss (SVM):** $\Phi(u) = \max(0, 1 - u)$
- ▶ **Logistic Loss:** $\Phi(u) = \log(1 + e^{-u})$
- ▶ **Exponential Loss (AdaBoost):** $\Phi(u) = e^{-u}$
- ▶ **Squared Loss:** $\Phi(u) = (1 - u)^2$



Risk Decomposition: Sources of Error

We consider loss functions that are defined for real-valued outputs (for binary classification problems we will use a surrogate loss).

For any ERM estimator $\hat{f} \in \mathcal{F}$ trained on N samples:

$$\mathbb{E}[R(\hat{f})] - R^* = \underbrace{\mathbb{E}[R(\hat{f})] - \inf_{f \in \mathcal{F}} R(f)}_{\text{Estimation Error}} + \underbrace{\inf_{f \in \mathcal{F}} R(f) - R^*}_{\text{Approximation Error}}$$

- ▶ **Approximation Error:** Fundamental limitation of the model class \mathcal{F}
 - ▶ How well can the *best possible* function in \mathcal{F} approximate f^* ?
 - ▶ Only reduced by choosing more flexible \mathcal{F} (more complex models)
 - ▶ Independent of sample size N
- ▶ **Estimation Error:** Error from finite sample learning
 - ▶ How much worse is our empirical solution \hat{f} vs. the best in class?
 - ▶ Decreases with more data (typically $O(1/\sqrt{N})$ or better)
 - ▶ Increases with model complexity (richer \mathcal{F})

Uniform Deviation

Estimation error is controlled by uniform deviation over the function class:

$$\mathbb{E}[R(\hat{f})] - \inf_{f \in \mathcal{F}} R(f) \leq 2\mathbb{E} \left[\sup_{f \in \mathcal{F}} |R(f) - \hat{R}(f)| \right]$$

Proposition 1: Application of McDiarmid's Inequality

Let $Z = \sup_{f \in \mathcal{F}} (R(f) - \hat{R}(f))$ where loss is bounded: $\ell(y, f(x)) \in [0, \ell_\infty]$. Then,

$$P(Z \geq \mathbb{E}[Z] + t) \leq \exp \left(-\frac{2Nt^2}{\ell_\infty^2} \right),$$

Proof.

See blackboard. □

The Problem: We still need to bound $\mathbb{E}[\sup_{f \in \mathcal{F}} |R(f) - \hat{R}(f)|]$. This is where Rademacher complexity comes in.

Rademacher Complexity: Definition

Definition 8: Rademacher Complexity

Consider N i.i.d. sample $z_1, \dots, z_N \in \mathcal{Z}$ and a class \mathcal{H} of functions from \mathcal{Z} to \mathbb{R} . The Rademacher complexity of \mathcal{H} is:

$$\mathcal{R}_N(\mathcal{H}) = \mathbb{E}_{\mathbf{z}, \varepsilon} \left[\sup_{h \in \mathcal{H}} \frac{1}{N} \sum_{i=1}^N \varepsilon_i h(z_i) \right]$$

where $\varepsilon_i \stackrel{\text{iid}}{\sim} \text{Rademacher}(\pm 1)$ are independent of the data.

- ▶ **Random Noise Test:** How well can functions in \mathcal{H} fit random noise (ε_i)?
- ▶ **Complexity Measure:** Rich function classes can fit noise well \Rightarrow high $\mathcal{R}_N(\mathcal{H})$
- ▶ **Sample Size Effect:** More data makes it harder to fit noise $\Rightarrow \mathcal{R}_N(\mathcal{H})$ typically decreases as N increases
- ▶ **Dimension Independent:** Often gives dimension-free bounds

Symmetrization: The Key Lemma

Connection to Generalization: Functions that can fit random noise well are prone to overfitting real data. Rademacher complexity quantifies this overfitting potential.

A useful lemma:

Lemma 1: Symmetrization Lemma

For any function class \mathcal{H} : $\mathbb{E} \left[\sup_{h \in \mathcal{H}} \left(\frac{1}{N} \sum_{i=1}^N h(z_i) - \mathbb{E}[h(Z)] \right) \right] \leq 2\mathcal{R}_N(\mathcal{H})$.

Proof.

See blackboard. □

Rademacher Generalization Bound

Theorem 1: Rademacher Generalization Bound

Let \mathcal{F} be a function class and ℓ be a loss function with $|\ell(y, f(x))| \leq M$. Define the loss function class $\mathcal{H} = \{(x, y) \mapsto \ell(y, f(x)) : f \in \mathcal{F}\}$. Then for any $\delta > 0$, with probability at least $1 - \delta$, $\sup_{f \in \mathcal{F}} (R(f) - \hat{R}(f)) \leq 2\mathcal{R}_N(\mathcal{H}) + M\sqrt{\frac{\log(1/\delta)}{2N}}$.

Proof.

See blackboard. □

Proposition 2: Contraction Principle

If $\ell(y, \cdot)$ is L -Lipschitz for each y , then for loss class $\mathcal{H} = \{\ell(\cdot, f(\cdot)) : f \in \mathcal{F}\}$, $\mathcal{R}_N(\mathcal{H}) \leq L \cdot \mathcal{R}_N(\mathcal{F})$.

Proof.

See blackboard. □

Rademacher Complexity: Key Properties

Proposition 3: Linear Functions

For $\mathcal{F} = \{f_\theta(x) = \theta^\top \phi(x) : \|\theta\|_2 \leq D\}$: $\mathcal{R}_N(\mathcal{F}) = \frac{D}{N} \mathbb{E} \left[\left\| \sum_{i=1}^N \varepsilon_i \phi(x_i) \right\|_2 \right]$
If $\mathbb{E}[\|\phi(X)\|_2^2] \leq R^2$, then: $\mathcal{R}_N(\mathcal{F}) \leq \frac{DR}{\sqrt{N}}$.

Proof.

See blackboard. □

💡 **Dimension-Free Bound:** The bound DR/\sqrt{N} does not depend on the dimension of $\phi(x)$! Applicable to infinite-dimensional spaces (e.g., RKHS).

Main Generalization Theorem

Theorem 2: Generalization Bound for Linear Predictors

Consider:

- ▶ Linear predictors: $\mathcal{F} = \{f_\theta(x) = \theta^\top \phi(x) : \|\theta\|_2 \leq D\}$
- ▶ Loss function is L -Lipschitz and bounded
- ▶ Bounded features: $\mathbb{E}[\|\phi(X)\|_2^2] \leq R^2$
- ▶ ERM estimator $\hat{f} = \arg \min_{f \in \mathcal{F}} \hat{R}(f)$

Then $\mathbb{E}[R(\hat{f})] - \inf_{f \in \mathcal{F}} R(f) \leq \frac{4LDR}{\sqrt{N}}$. Moreover, for any $\delta > 0$, with probability $\geq 1 - \delta$, $R(\hat{f}) - \inf_{f \in \mathcal{F}} R(f) \leq \frac{4LDR}{\sqrt{N}} + \ell_\infty \sqrt{\frac{\log(1/\delta)}{2N}}$.

Proof.

See blackboard. □

- ▶ Rate $O(1/\sqrt{N})$ is **minimax optimal** for this setting
- ▶ Bound scales with $L \cdot D \cdot R$ (loss smoothness \times model complexity \times data scale)
- ▶ **Dimension-free:** Works for infinite-dimensional $\phi(x)$ (kernels!)
- ▶ Others: VC dimension bound, PAC-Bayes bound (not covered)

Vapnik-Chervonenkis (VC) Dimension

For classification models, the VC dimension provides a theoretical measure of model complexity, or the "richness" of the hypothesis class \mathcal{F} .

Definition 9: Shattering and VC Dimension

A class of functions \mathcal{F} **shatters** a set of N points if it can realize every possible binary labeling of those points. The **VC dimension** h of \mathcal{F} is the maximum number of points that can be shattered.

The VC dimension provides a probabilistic upper bound on the true risk:

$$R(\hat{f}) \leq \hat{R}_N(\hat{f}) + \sqrt{\frac{h(\log(2N/h)+1) - \log(\eta/4)}{N}}$$

⚠ This bound is often too loose for practical model selection but is of great theoretical importance.

Theoretical vs Practical: Bridging the Gap

Practical Tools:

- ▶ **Cross-validation** works broadly without strong assumptions
- ▶ **Information criteria** efficient for likelihood-based models
- ▶ **Bootstrap** provides flexible uncertainty quantification
- ▶ **Nested CV** prevents selection bias in assessment

Theoretical Insights:

- ▶ **Convex surrogates** make hard problems tractable
- ▶ **Rademacher complexity** gives dimension-free generalization bounds
- ▶ **Regularization** can improve rates from $O(1/\sqrt{N})$ to $O(1/N)$
- ▶ **Linear models** have strong theoretical guarantees

Key Takeaways

- ▶ **Practice:** Cross-validation, AIC/BIC, bootstrap give usable estimates of test error.
- ▶ **Theory:** Statistical learning theory explains why generalization is possible.
- ▶ Both perspectives are complementary:
 - ▶ Empirical tools guide model selection.
 - ▶ Theoretical tools justify and bound their performance.

💡 **Controlling generalization error = unifying theme.**

Exercise 7

1. **Train Error is Smaller Than Test Error, On Average.** Solve Exercise 2.9 in ESL.
2. **Best Subset Analysis.** Solve Exercise 7.9 in ESL.
3. **Calibration.** Show that the logistic loss and the exponential loss are calibrated. Construct an example of a non-calibrated surrogate loss.
4. **Rademacher Complexity.** Solve Exercise 4.8 in Bach.
5. **Generalization Bound for Kernel Methods.** Extend Theorem 2 to kernel methods.