# Generalization and Model Selection
# The Story of Empirical Risk vs True Risk

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Machine Learning 10-701

# Overview

1. True risk vs. empirical risk
2. Improving empirical risk minimization
3. Model selection (which requires estimating true risk **of estimators**)
4. Estimating true risk of estimators
5. Analyzing generalization error via true risk

# 1. TRUE RISK VS EMPIRICAL RISK

# True Risk vs. Empirical Risk

True Risk: Target performance measure

Classification – Probability of misclassification $P(f(X) \neq Y)$

Regression – Mean Squared Error $\mathbb{E}[(f(X) - Y)^2]$

Expected performance on a random test point (X,Y)

# True Risk vs. Empirical Risk

True Risk: Target performance measure

Classification – Probability of misclassification $P(f(X) \neq Y)$

Regression – Mean Squared Error $\mathbb{E}[(f(X) - Y)^2]$

Expected performance on a random test point (X,Y)

Empirical Risk: Performance on training data

Classification – Proportion of misclassified examples $\frac{1}{n}\sum_{i=1}^{n} 1_{f(X_i) \neq Y_i}$

Regression – Average Squared Error $\frac{1}{n}\sum_{i=1}^{n} (f(X_i) - Y_i)^2$

# Some quick notation

$$\text{True Risk}: R(f) := \mathbb{E}(\ell(f(X), Y))$$

$$\text{Empirical Risk given data D}: \widehat{R}_D(f) := \frac{1}{|D|} \sum_{i \in D} \ell(f(X_i), Y_i)$$

# True Risk vs Empirical Risk

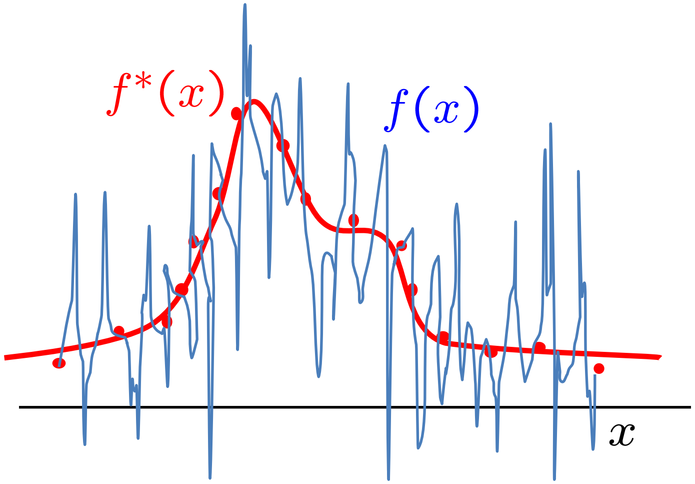
- So we minimize with respect to empirical risk
- And evaluate with respect to true risk

- Is there any danger to this mismatch?
  - Overfitting!!

# Overfitting

Is the following predictor a good one?

$$f(x) = \begin{cases} Y_i, & x = X_i \text{ for } i = 1, \ldots, n \\ \text{any value}, & \text{otherwise} \end{cases}$$




What is its empirical risk? (performance on training data)

zero !

What about true risk?

>> zero

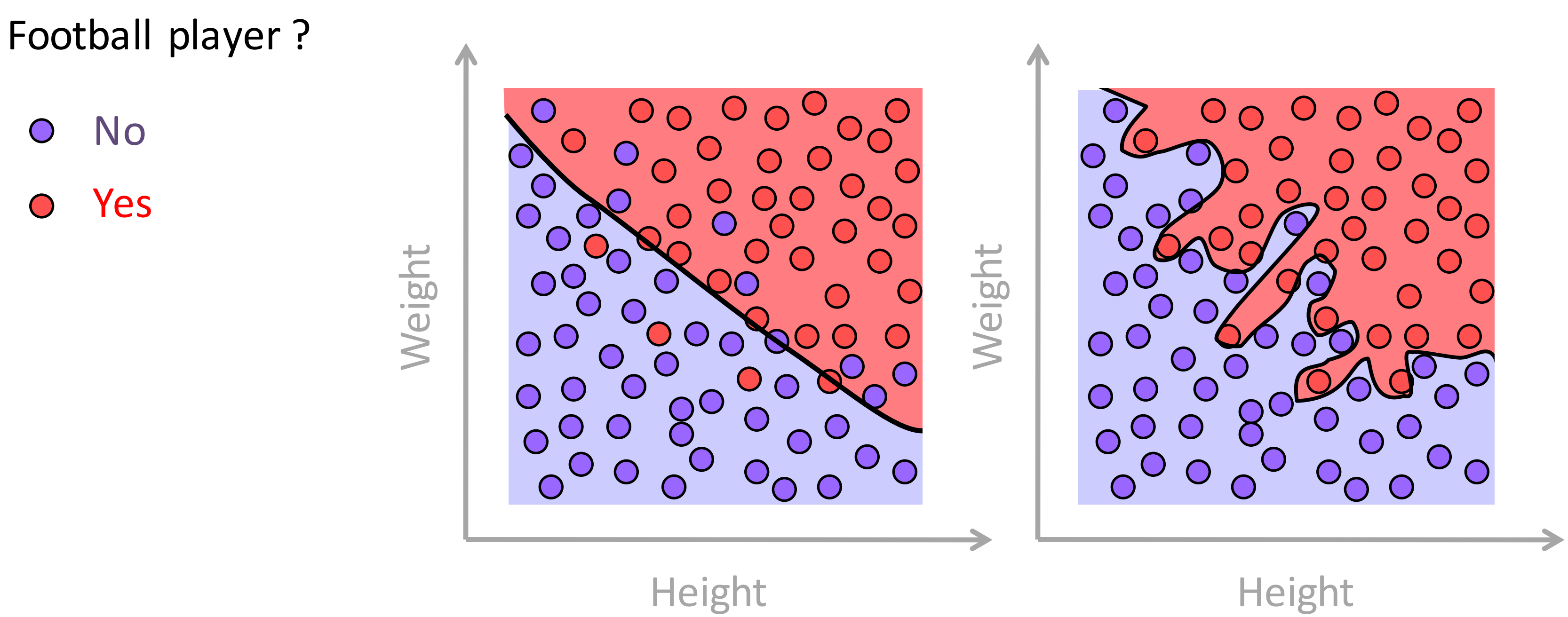
Will predict very poorly on new random test point:

Large generalization error !

# Overfitting

If we allow very complicated predictors, we could overfit the training data.

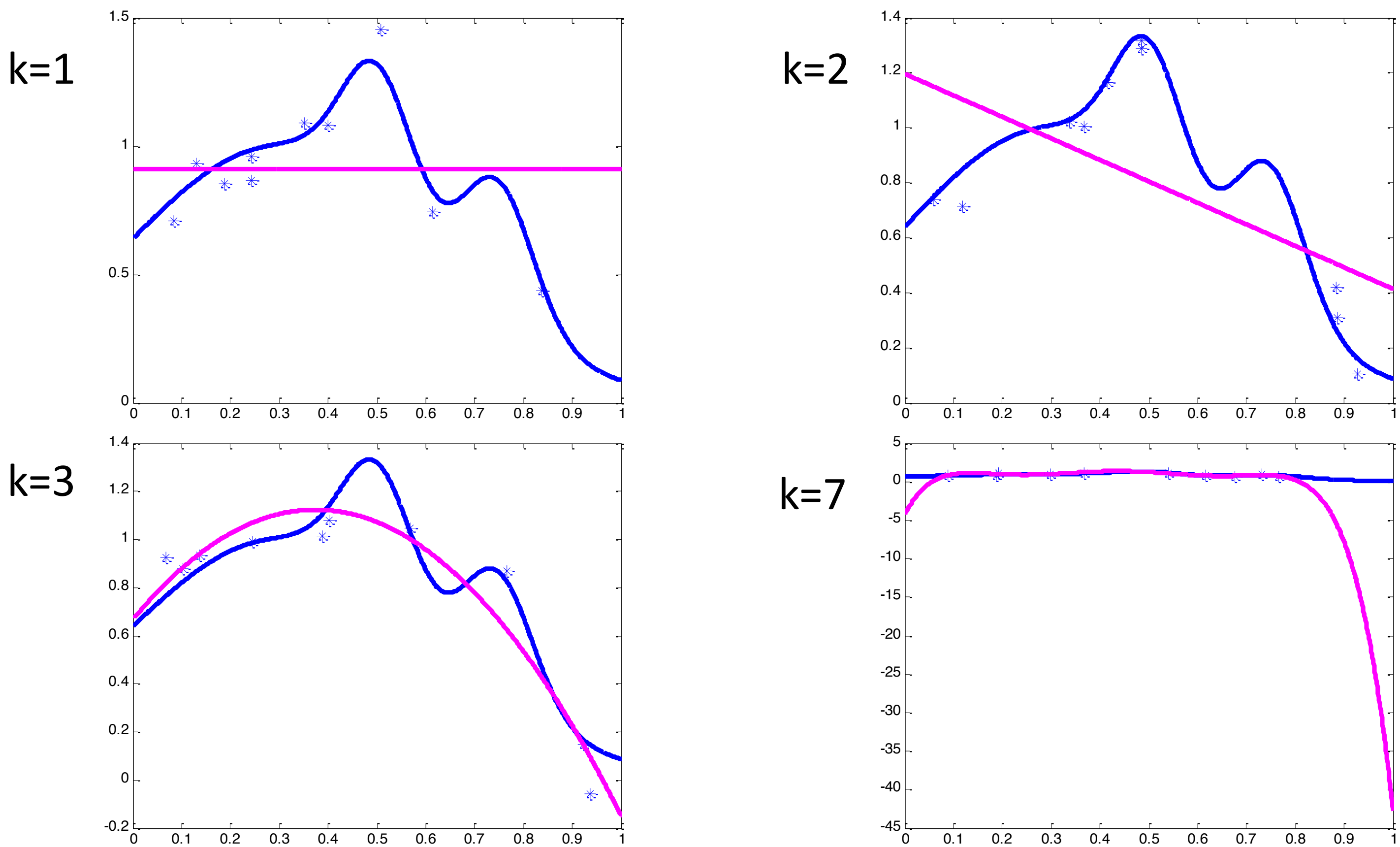
Examples: Classification (0-NN classifier)



# Overfitting

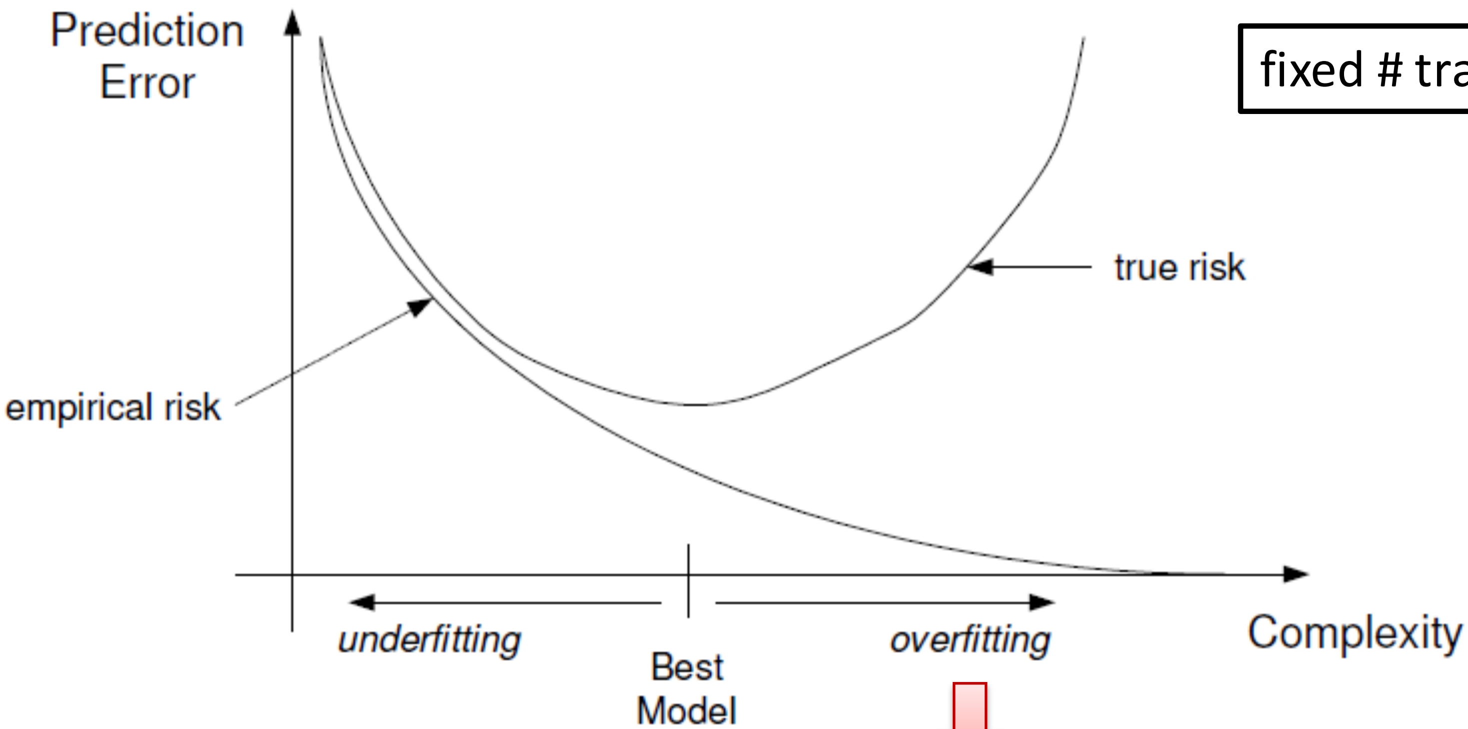
If we allow very complicated predictors, we could overfit the training data.

Examples: Regression (Polynomial of order k – degree up to k-1)



# Overfitting: Effect of discrepancy between empirical and true risks

If we allow very complicated predictors, we could overfit the training data.




fixed # training data

Empirical risk is no longer a good indicator of true risk

# Questions

- So, Empirical risk minimization (ERM) might "overfit" when the model complexity is high, due to mismatch between empirical risk and true risk
- But we do not have access to true risk since it depends on unknown distribution :(
- And so we estimate true risk via empirical risk!
- **Can we do better?**

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# 2. IMPROVING EMPIRICAL RISK MINIMIZATION

# Risk Minimization

- Can we improve upon ERM by using better estimates of true risk than empirical risk?

# Structural Risk Minimization

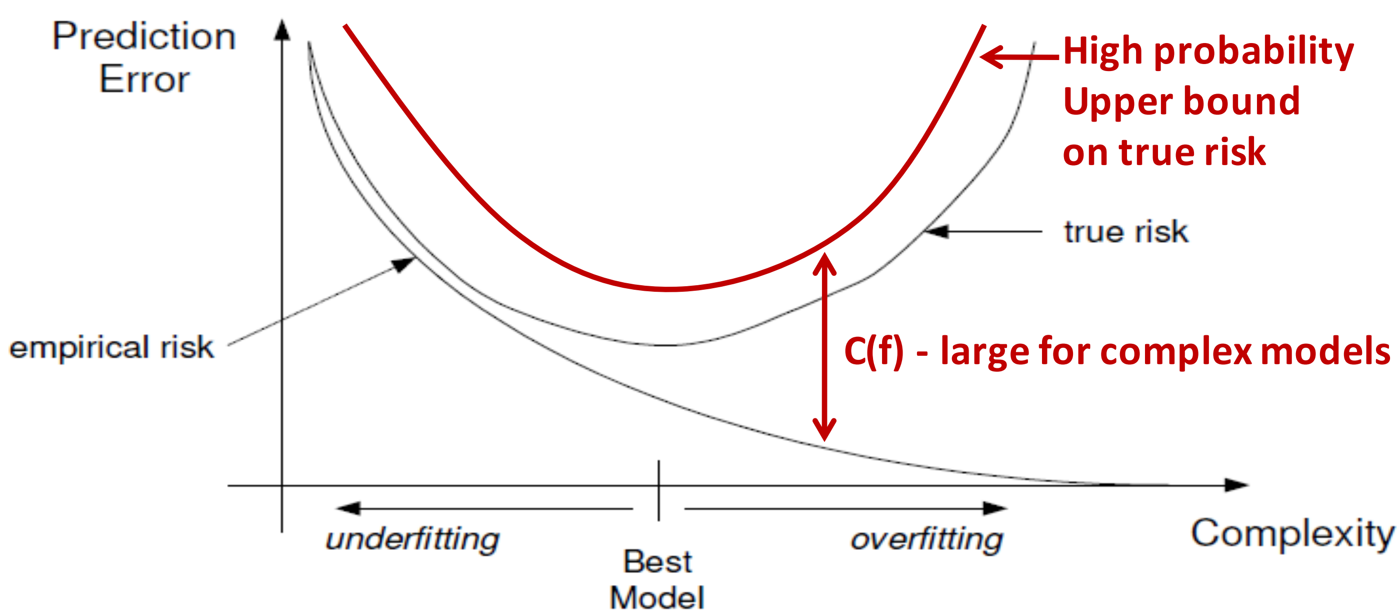
Penalize models using bound on **deviation of true and empirical risks**.

$$\widehat{f}_n \quad = \quad \arg\min_{f \in \mathcal{F}} \left\{ \widehat{R}_n(f) + C(f) \right\}$$

Bound on deviation from true risk

With high probability, $|R(f) - \widehat{R}_n(f)| \leq C(f) \quad \forall f \in \mathcal{F}$

Concentration bounds (later)



# Structural Risk Minimization

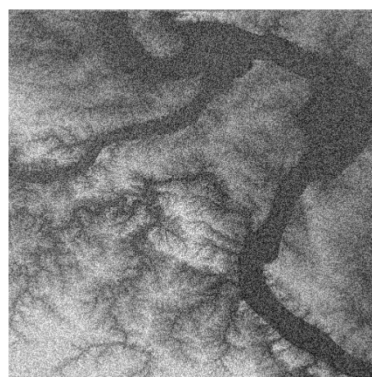
Deviation bounds are typically pretty loose, for small sample sizes. In practice,

$$\widehat{f}_n = \arg\min_{f \in \mathcal{F}} \left\{ \widehat{R}_n(f) + \lambda C(f) \right\}$$

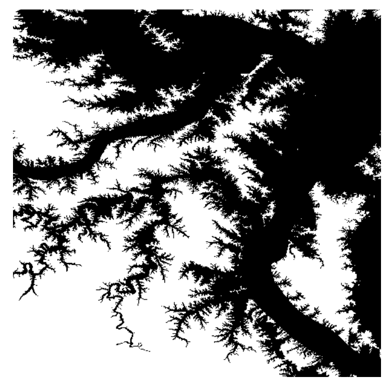
$\lambda$ → Choose by **model selection**!

Problem: Identify flood plain from noisy satellite images

Noiseless image



Noisy image



True Flood plain
(elevation level > x)

# Structural Risk Minimization

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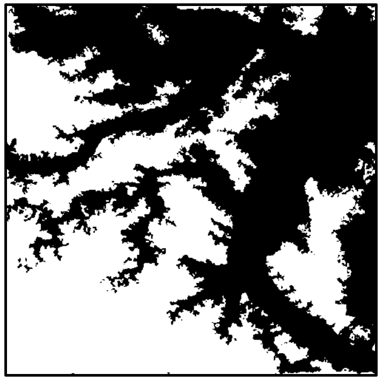
→ Choose by **model selection!**

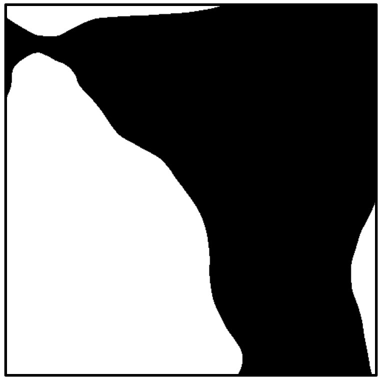
Problem: Identify flood plain from noisy satellite images

True Flood plain
(elevation level > x)

Zero penalty



CV penalty

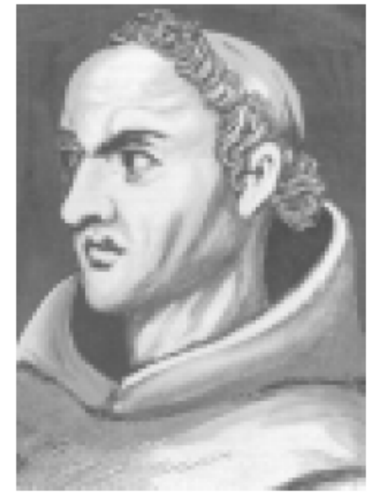


Theoretical penalty

# Occam's Razor

William of Ockham (1285-1349) *Principle of Parsimony:*

"One should not increase, beyond what is necessary, the number of entities required to explain anything."

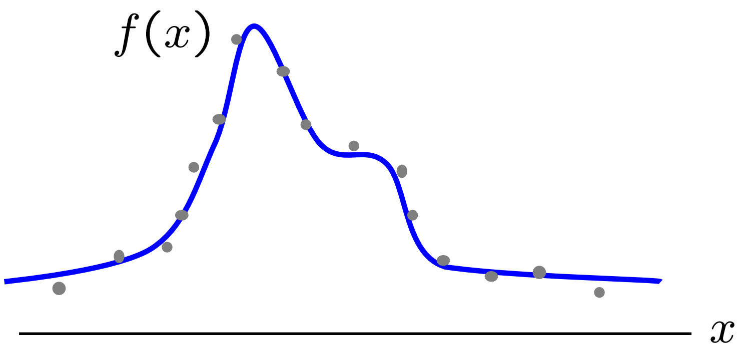


Alternatively, seek the simplest explanation.

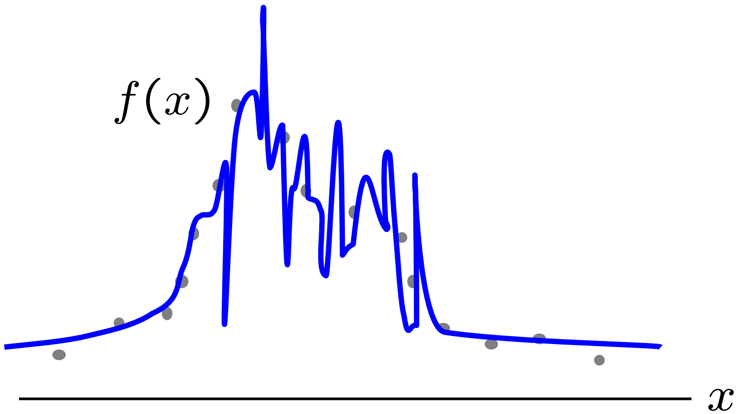
Penalize complex models based on

- Prior information (bias)
- Information Criterion (MDL, AIC, BIC)

# Importance of Domain Knowledge




Oil Spill Contamination




Distribution of photon arrivals

Compton Gamma-Ray Observatory Burst and Transient Source Experiment (BATSE)

# Complexity Regularization

Penalize complex models using **prior knowledge**.

$$\widehat{f}_n = \arg\min_{f \in \mathcal{F}} \left\{ \widehat{R}_n(f) + C(f) \right\}$$

Cost of model
(log prior)

Bayesian viewpoint:

prior probability of *f*, p*(f)* ≡ $e^{-C(f)}$

cost is small if *f* is highly probable, cost is large if *f* is improbable

ERM (empirical risk minimization) over a restricted class *F*
≡ uniform prior on *f* ϵ *F*, zero probability for other predictors

$$\widehat{f}_n^L = \arg\min_{f \in \mathcal{F}_L} \widehat{R}_n(f)$$

# Complexity Regularization

Penalize complex models using **prior knowledge**.

$$\widehat{f}_n = \arg\min_{f\in\mathcal{F}} \left\{ \widehat{R}_n(f) + C(f) \right\}$$

Cost of model
(log prior)

Examples: MAP estimators
Regularized Linear Regression - Ridge Regression, Lasso

$$\widehat{\theta}_{\text{MAP}} = \arg\max_{\theta} \log p(D|\theta) + \log p(\theta)$$

$$\widehat{\beta}_{\text{MAP}} = \arg\min_{\beta} \sum_{i=1}^{n} (Y_i - X_i\beta)^2 + \lambda ||\beta||$$

Penalize models based on some norm of regression coefficients

How to choose tuning parameter λ? **Model Selection**

# Information Criteria – AIC, BIC

Penalize complex models based on their **information content**.

$$\widehat{f}_n = \arg\min_{f \in \mathcal{F}} \left\{ \widehat{R}_n(f) + C(f) \right\}$$

→ # bits needed to describe *f* (description length)

**AIC (Akiake IC)** C(*f*) = # parameters

Allows # parameters to be infinite as # training data n become large

**BIC (Bayesian IC)** C(*f*) = # parameters * log n

Penalizes complex models more heavily – limits complexity of models as # training data n become large

# 3. MODEL SELECTION

# Model Selection

- Model classes with increasing complexity
  - Regularization parameter λ in structural risk estimators
    - Larger values of λ => Lower complexity
    - Question: How to select λ?
  - Regression with polynomials of order k = 0, 1, 2, …
    - Higher degree => Higher complexity
    - Question: How to select k?
  - k and λ are called "tuning" parameters

- General setup:
  - Define a finite set of model classes
    - Regression: $\{\mathcal{F}_{k=0}, \mathcal{F}_{k=1}, \mathcal{F}_{k=2}\}$
    - Structural risk: $\{\mathcal{F}_{\lambda=0.01}, \mathcal{F}_{\lambda=0.1}, \mathcal{F}_{\lambda=1}\}$
  - For each model class, find best estimator in model class, and estimate corresponding true risks: $\{\hat{R}(\hat{f}_1), \hat{R}(\hat{f}_2), \hat{R}(\hat{f}_3)\}$

  - Model selection: Select best model class: $\arg\min_i \hat{R}(\hat{f}_i)$

# Model Selection

Formal setup:

Model Classes $\{\mathcal{F}_\lambda\}_{\lambda \in \Lambda}$ of increasing complexity $\mathcal{F}_1 \prec \mathcal{F}_2 \prec \ldots$

$$\min_{\lambda} \min_{f \in \mathcal{F}_\lambda} J(f, \lambda)$$

Stage I: *Given* λ, estimate $\hat{f}_\lambda$ using

- Empirical risk minimization
- Structural risk minimization
- Complexity regularized risk minimization

Stage II: *Select* λ for which $\hat{f}_\lambda$ has minimum value of true risk estimated using

- **Cross-validation**
- **Hold-out**
- **Information-theoretic risk estimates (AIC, BIC)**

# 4. ESTIMATING TRUE RISK OF ESTIMATORS

# Estimating True Risk of Estimators

- Suppose we train an estimator $\widehat{f}_D$ on data D
- How do we estimate its true risk $R(\widehat{f}_D)$ ?
- We could use the training data D itself i.e. use empirical risk on training data $\widehat{R}_D(\widehat{f}_D)$
- Not such a good idea
- If the midterm questions are comprised entirely of homework questions, would the midterm grade be an optimistic estimate of the "true" midterm grade?
  - Yes!
- Similarly, using the empirical risk on training data would be an optimistic estimate of the true risk

# Algorithmic and Closed Form Estimates of True Risk

- Algorithmic Estimates of True Risk:
  - Empirical Risk
    - Optimistic
  - Evaluating Risk on a holdout set
  - Cross-validation
- Closed form Estimates of True Risk
  - Structural Risk

# Hold-out method

Can judge generalization error by using an independent sample of data.

Hold – out procedure:

n data points available $D \equiv \{X_i, Y_i\}_{i=1}^n$

1) Split into two sets: Training dataset Holdout dataset

$$D_T = \{X_i, Y_i\}_{i=1}^m \qquad D_V = \{X_i, Y_i\}_{i=m+1}^n$$

2) Use $D_T$ for training a predictor $\widehat{f}_{D_T}$

3) Use $D_V$ for evaluating the predictor

$$\widehat{R}_{D_V}(\widehat{f}_{D_T})$$

# Hold-out method

Drawbacks:

- May not have enough data to afford setting one subset aside for getting a sense of generalization abilities
- Holdout error may be misleading (bad estimate of generalization error) if we get an "unfortunate" split

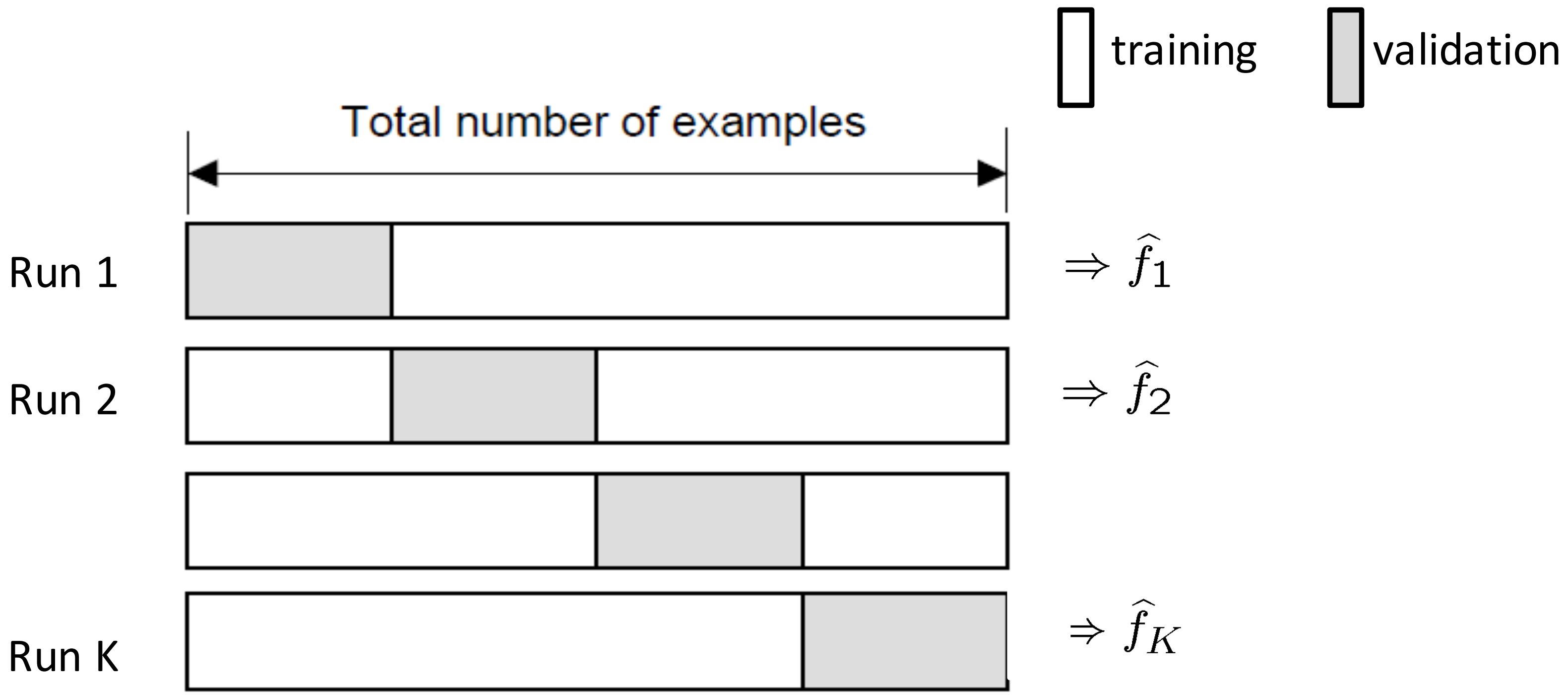
# Cross-validation

K-fold cross-validation

Create K-fold partition of the dataset.

Form K hold-out predictors, each time using one partition as validation and rest K-1 as training datasets.

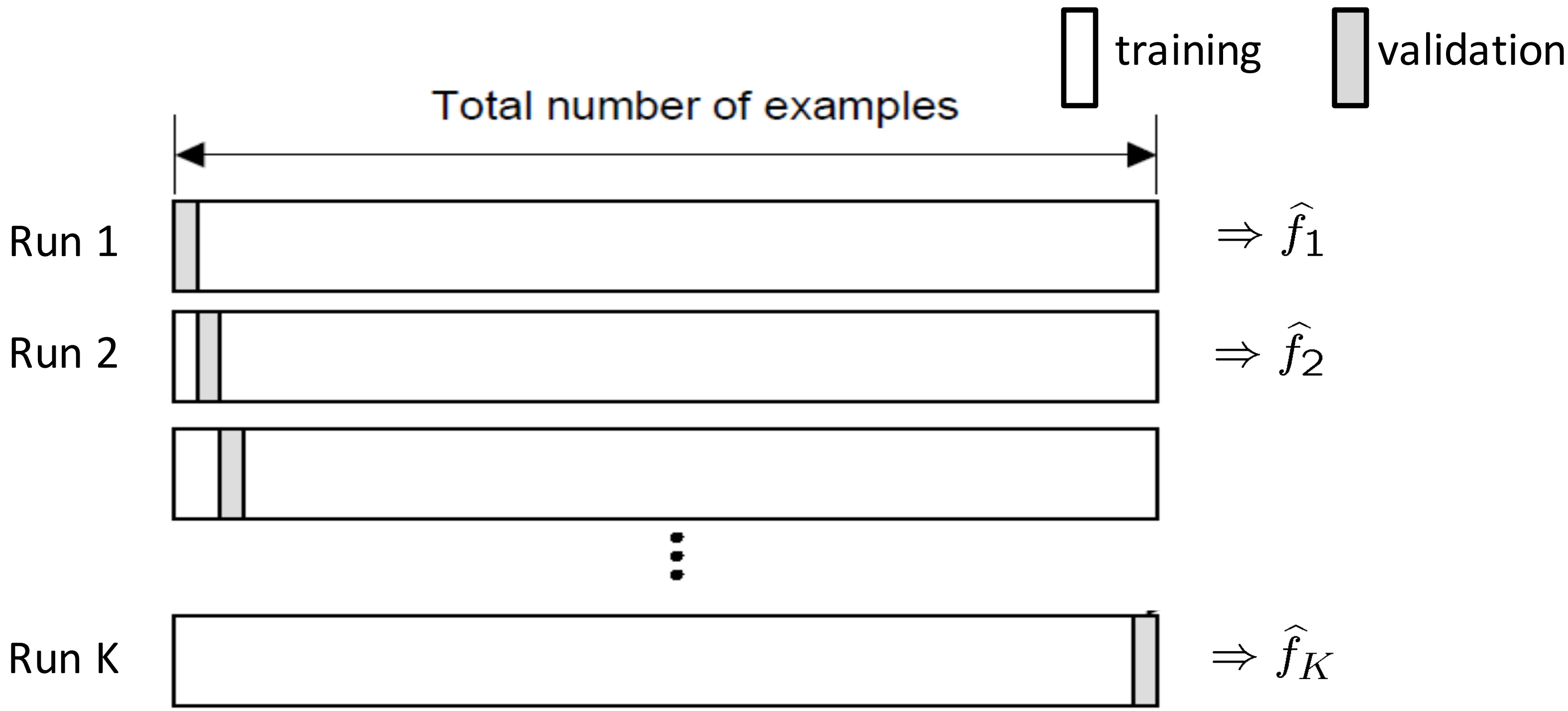
Final predictor is average/majority vote over the K hold-out estimates.



# Cross-validation

Leave-one-out (LOO) cross-validation

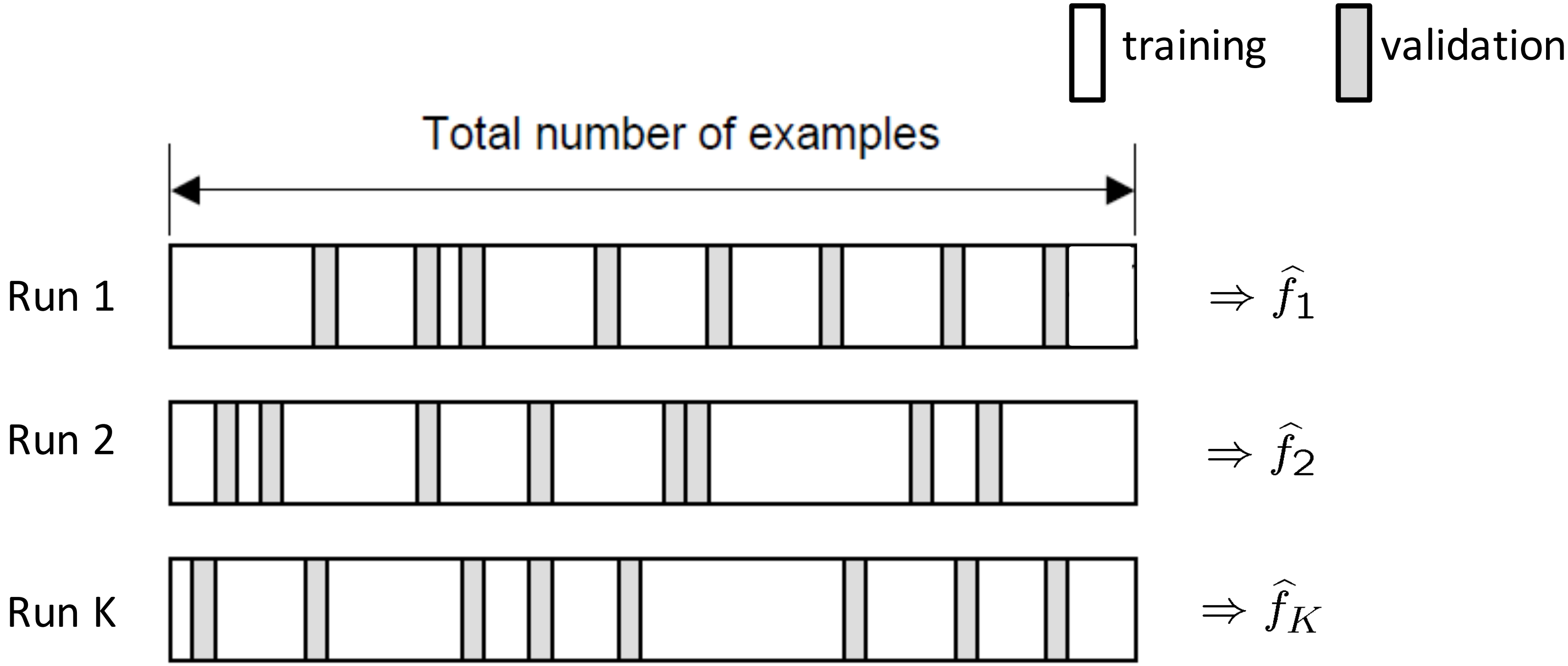
Special case of K-fold with K=n partitions
Equivalently, train on n-1 samples and validate on only one sample per run for n runs



# Cross-validation

## Random subsampling

Randomly subsample a fixed fraction $\alpha n$ (0< $\alpha$ <1) of the dataset for validation.
Form hold-out predictor with remaining data as training data.
Repeat K times
Final predictor is average/majority vote over the K hold-out estimates.



# Estimating true risk

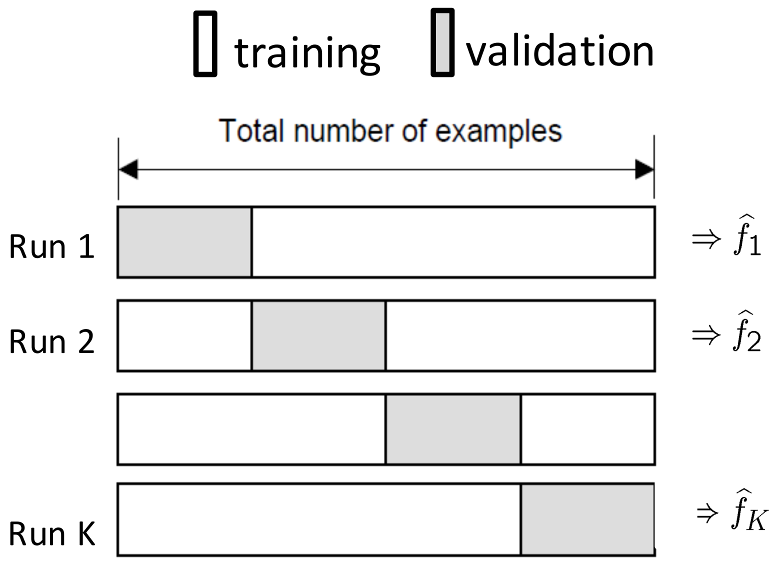
K-fold/LOO/random sub-sampling:

Error estimate = $\frac{1}{K}\sum_{k=1}^{K}\widehat{R}_{V_k}(\widehat{f}_{T_k})$

We want to estimate the error of a predictor based on n data points.

If K is large (close to n), bias of error estimate is small since each training set has close to n data points.

However, variance of error estimate is high since each validation set has fewer data points and $\widehat{R}_{V_k}$ might deviate a lot from the mean.



# Practical Issues in Cross-validation

How to decide the values for $K$ and $\alpha$ ?

- Large K
  + The bias of the error estimate will be small
  - The variance of the error estimate will be large (few validation pts)
  - The computational time will be very large as well (many experiments)

- Small K
  + The # experiments and, therefore, computation time are reduced
  + The variance of the error estimate will be small (many validation pts)
  - The bias of the error estimate will be large

Common choice: K = 10, $\alpha$ = 0.1 ☺

# Structural Risk

**Add a penalty based on deviation of true and empirical risks**:

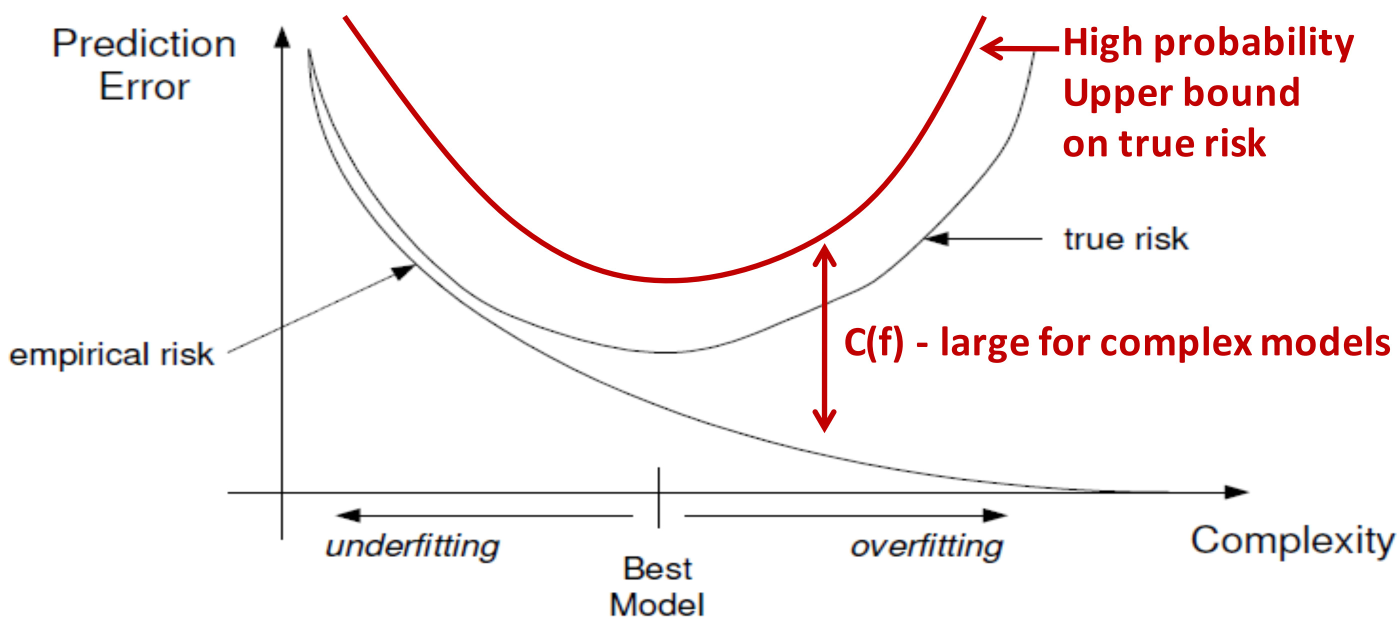
Suppose we have a bound, that with high probability:

$$|R(f) - \widehat{R}_n(f)| \leq C(f) \quad \forall f \in \mathcal{F}$$

$$R(f) \leq \widehat{R}_n(f) + C(f), \quad \forall f \in \mathcal{F}$$

Concentration bounds (later)

Use $\widehat{R}_n(\widehat{f}_n) + C(\widehat{f}_n)$ as a *pessimistic* estimate of true risk!



# 5. ANALYZING GENERALIZATION ERROR VIA TRUE RISK

# Estimation and Approximation Errors

$$\text{Estimated Predictor} : \widehat{f}_n$$

$$\text{Optimal Predictor} : f^*$$

$$\text{Risk of Estimated Predictor} : R(\widehat{f}_n)$$

$$\text{Above is random due to samples in training data}$$

$$\text{Expectation of above wrt training data} : \mathbb{E}(R(\widehat{f}_n))$$

$$\text{Risk of Optimal Predictor} : R(f^*)$$

# Players in the risk minimization story

Estimated Predictor : $\widehat{f}_n$

Optimal Predictor : $f^*$

Risk of Estimated Predictor : $R(\widehat{f}_n)$

Above is random due to samples in training data

Expectation of above wrt training data : $\mathbb{E}(R(\widehat{f}_n))$

Risk of Optimal Predictor : $R(f^*)$

Interested in the excess risk: $\mathbb{E}(R(\widehat{f}_n)) - R(f^*)$

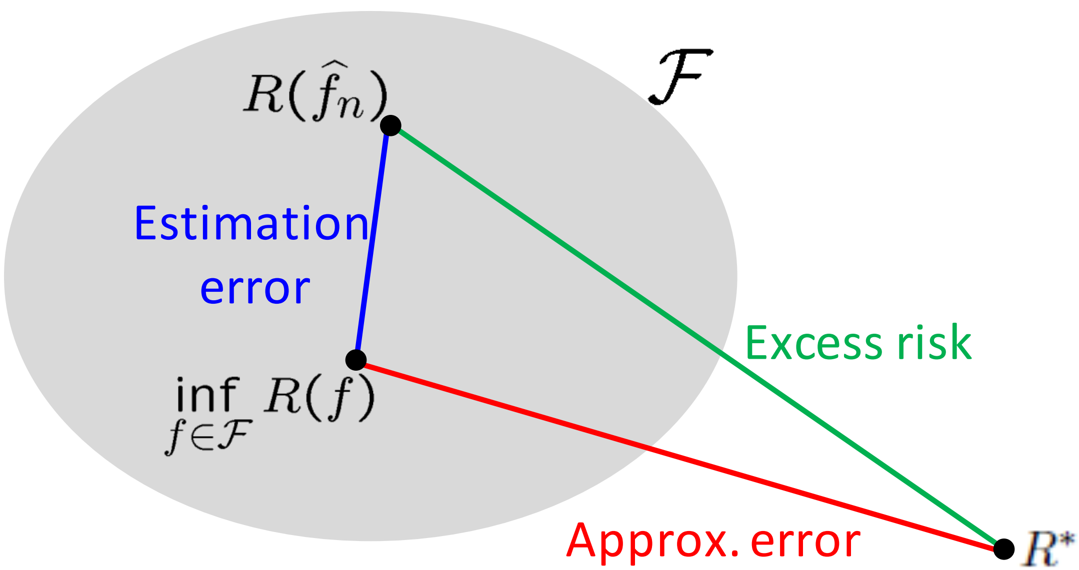
# Behavior of True Risk

Want $\widehat{f}_n$ to be as good as optimal predictor $f^*$

Excess Risk
$$E\left[R(\widehat{f}_n)\right] - R^* = \underbrace{\left(E[R(\widehat{f}_n)] - \inf_{f\in\mathcal{F}} R(f)\right)}_{\text{estimation error}} + \underbrace{\left(\inf_{f\in\mathcal{F}} R(f) - R^*\right)}_{\text{approximation error}}$$

**finite sample size + noise** ← Due to randomness of training data

Due to restriction of model class

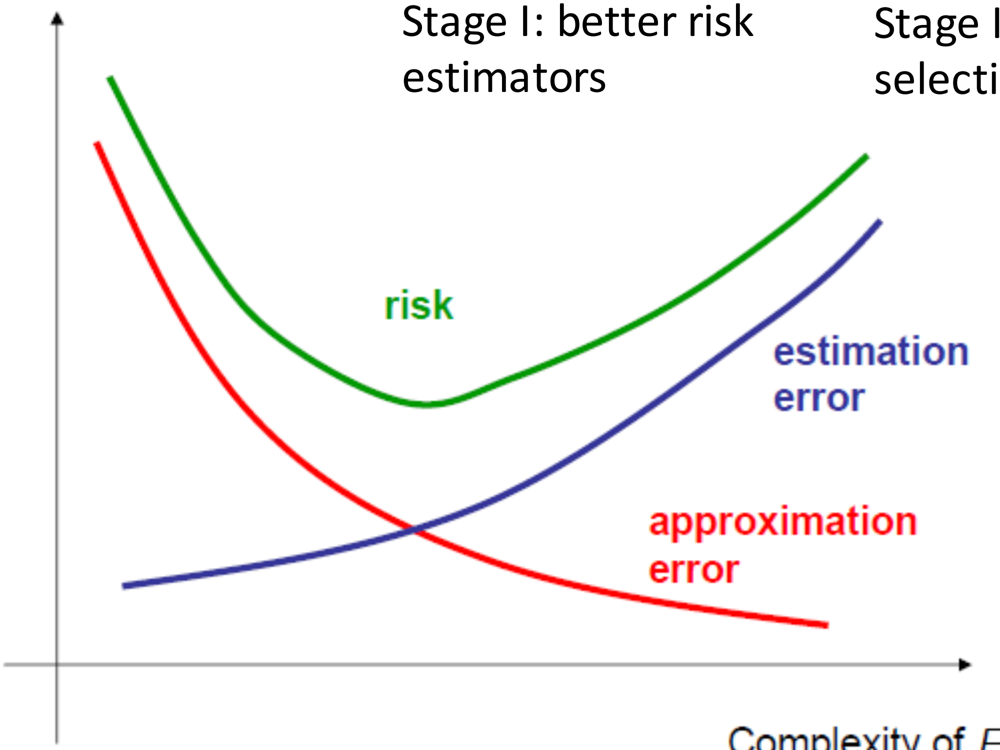


# Behavior of True Risk

$$E\left[R(\widehat{f}_n)\right] - R^* = \underbrace{\left(E[R(\widehat{f}_n)] - \inf_{f \in \mathcal{F}} R(f)\right)}_{\text{estimation error}} + \underbrace{\left(\inf_{f \in \mathcal{F}} R(f) - R^*\right)}_{\text{approximation error}}$$

Stage I: better risk estimators

Stage II: model selection



# Overview

1. True Risk vs. Empirical Risk
   - Explanation for overfitting
2. Improving Empirical Risk Minimization
   - Structural risk estimation (upper bound on true risk)
   - Complexity regularization (prior information, information criteria)
3. Estimating True Risk of Estimators
   - Algorithmic Estimators: Hold-out, Cross Validation
   - Closed-Form Estimators: Structural Risk
4. Model Selection by Estimating True Risk
   - *Given* complexity, estimate predictor
   - *Select* complexity based on estimates of true risk (HO, CV, etc.)
5. Analyzing Generalization Error via True Risk
   - Estimation error vs approximation error