Generalization, Model Selection

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True 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 vs. Empirical Risk

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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 $\frac{1}{n}\sum_{i=1}^{n} (f(X_i) - Y_i)^2$

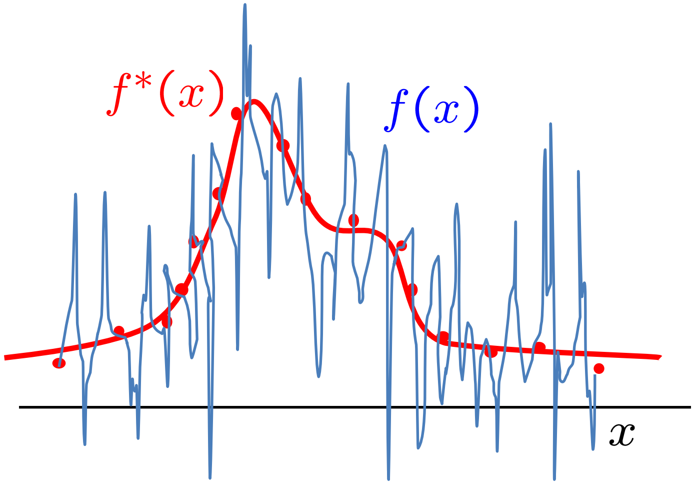
Some quick notation

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

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

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

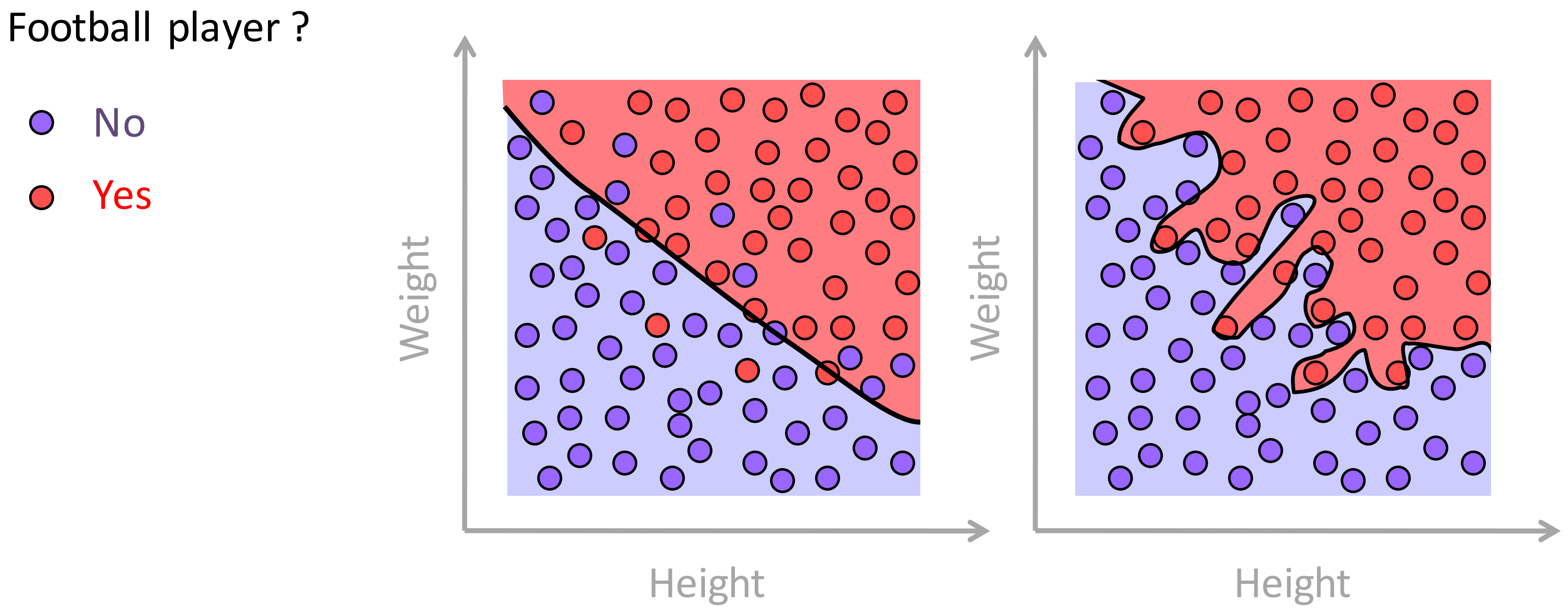
Will predict very poorly on new random test point:

Large generalization error !

Overfitting

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

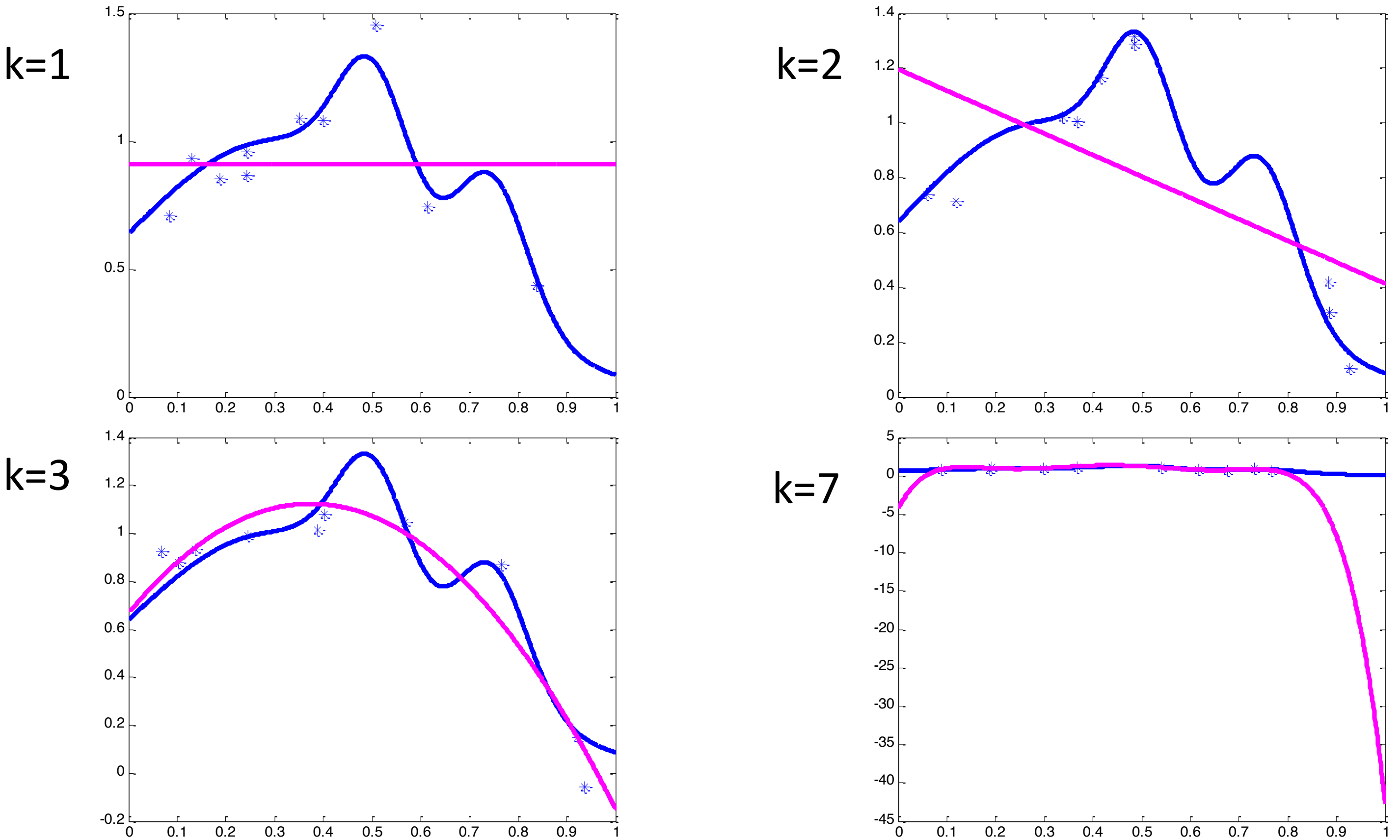
Examples: Classification (0-NN classifier)



Overfitting

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

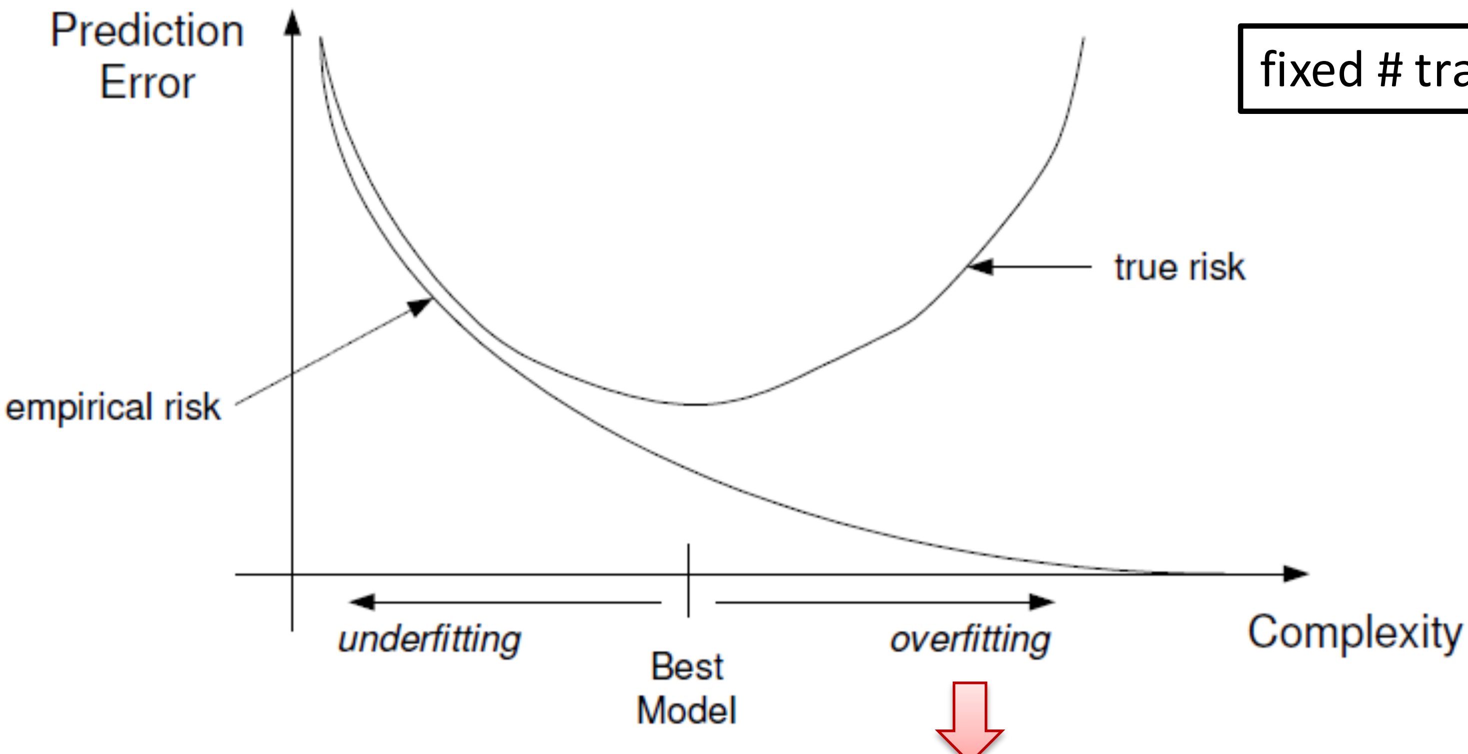
Examples: Regression (Polynomial of order k – degree up to k-1)



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

WE COULD ASK HOW TO COME UP WITH AN ESTIMATOR TO PREVENT OVERFITTING?

EASIER QUESTION: GIVEN EXISTING ESTIMATOR F, HOW SHOULD WE ESTIMATE ITS “TRUE RISK”?

Estimating True Risk

- 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?
- 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

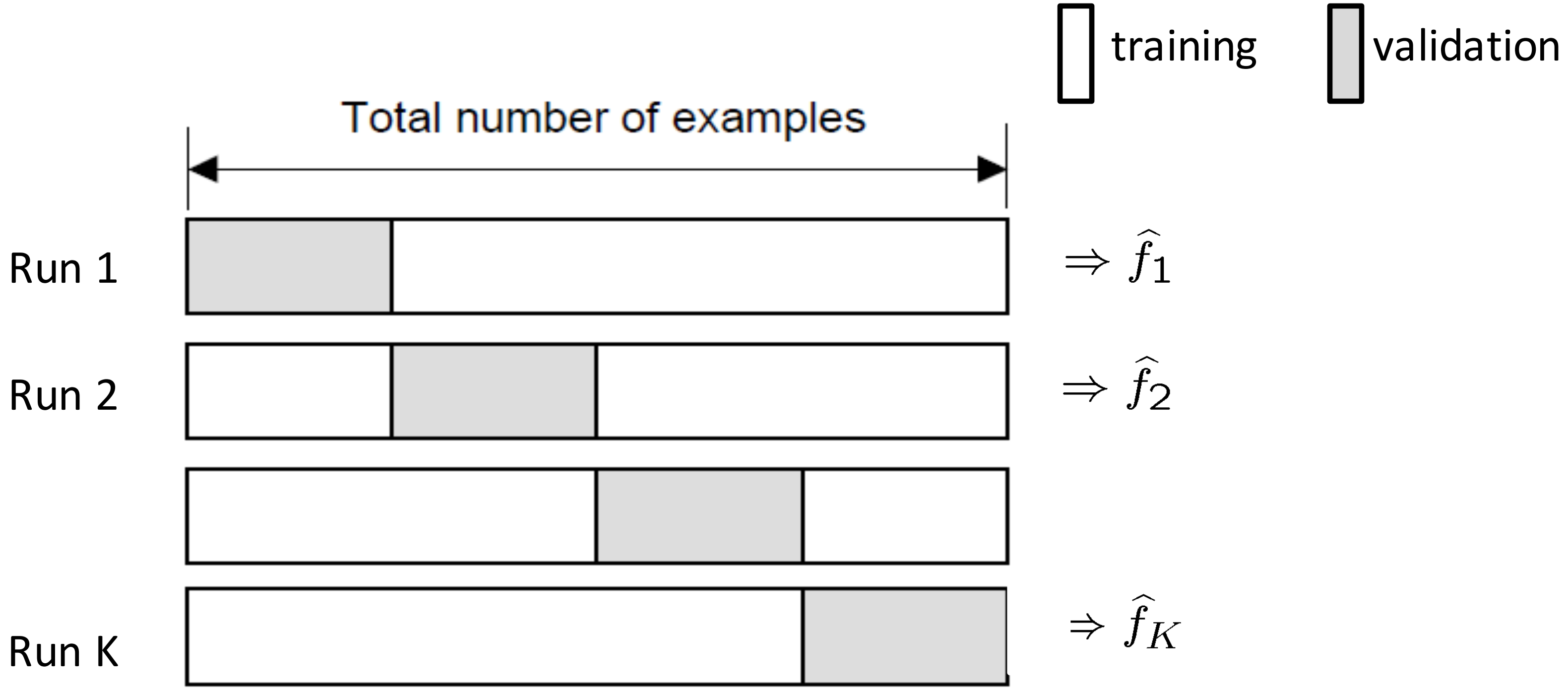
Drawbacks:

- 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

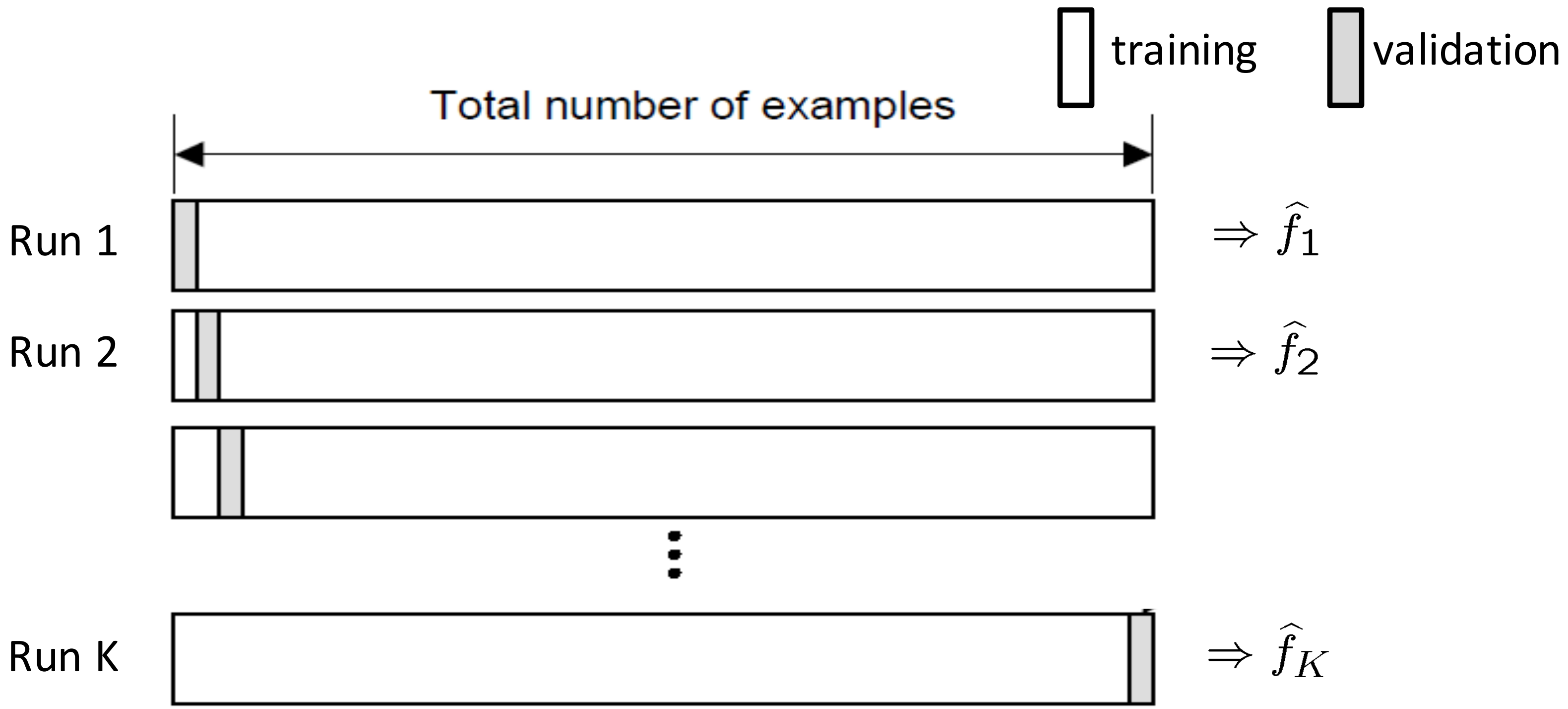
Create K-fold partition of the dataset.
Form K hold-out predictors, each time using one partition as validation and rest K-1 as training datasets.
Final predictor is average/majority vote over the K hold-out estimates.



Cross-validation

Leave-one-out (LOO) cross-validation

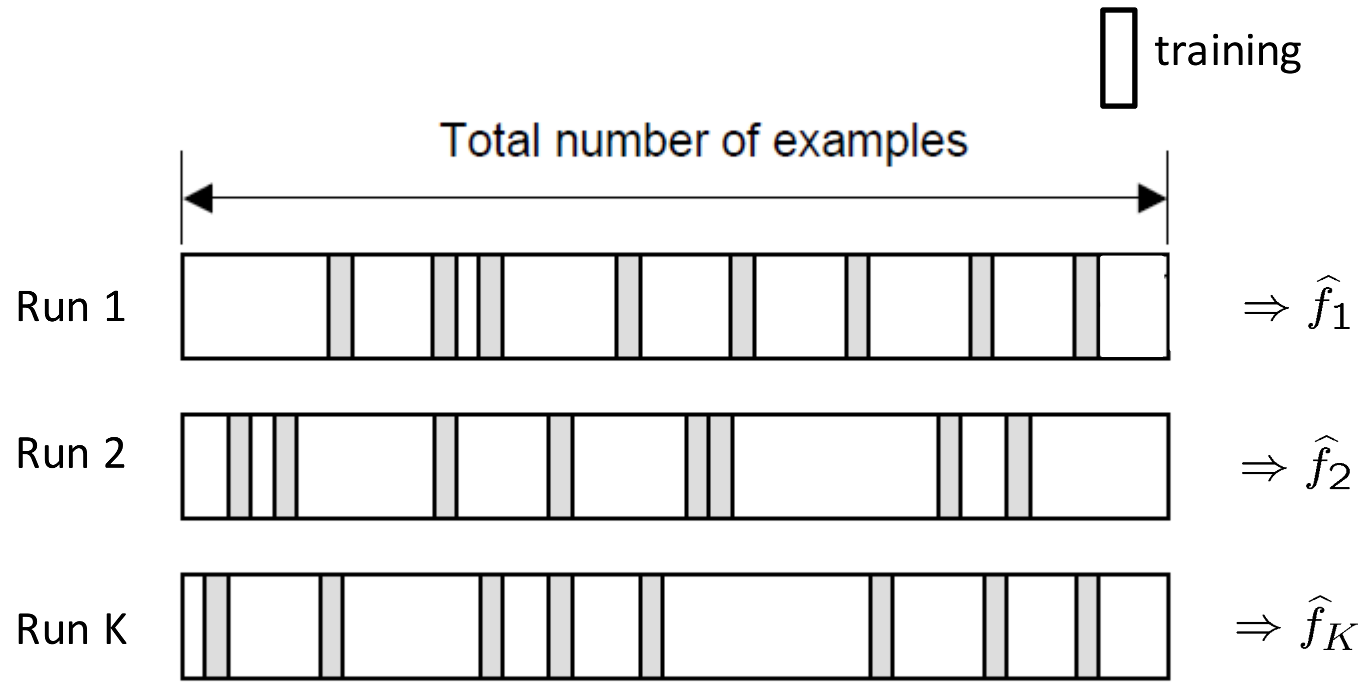
Special case of K-fold with K=n partitions
Equivalently, train on n-1 samples and validate on only one sample per run for n runs



Cross-validation

<u>Random subsampling</u>

Randomly subsample a fixed fraction αn ($0 < \alpha < 1$) 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

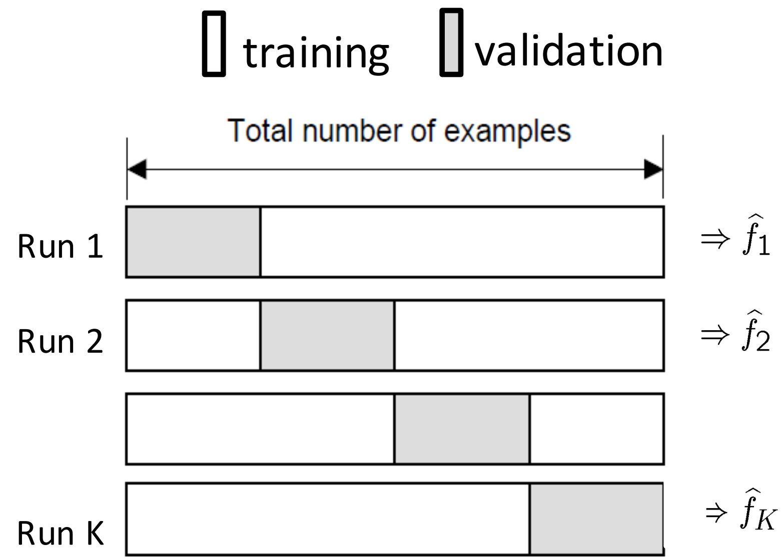
K-fold/LOO/random sub-sampling:

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 α ?

- 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, α = 0.1 ☺

Structural Risk

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

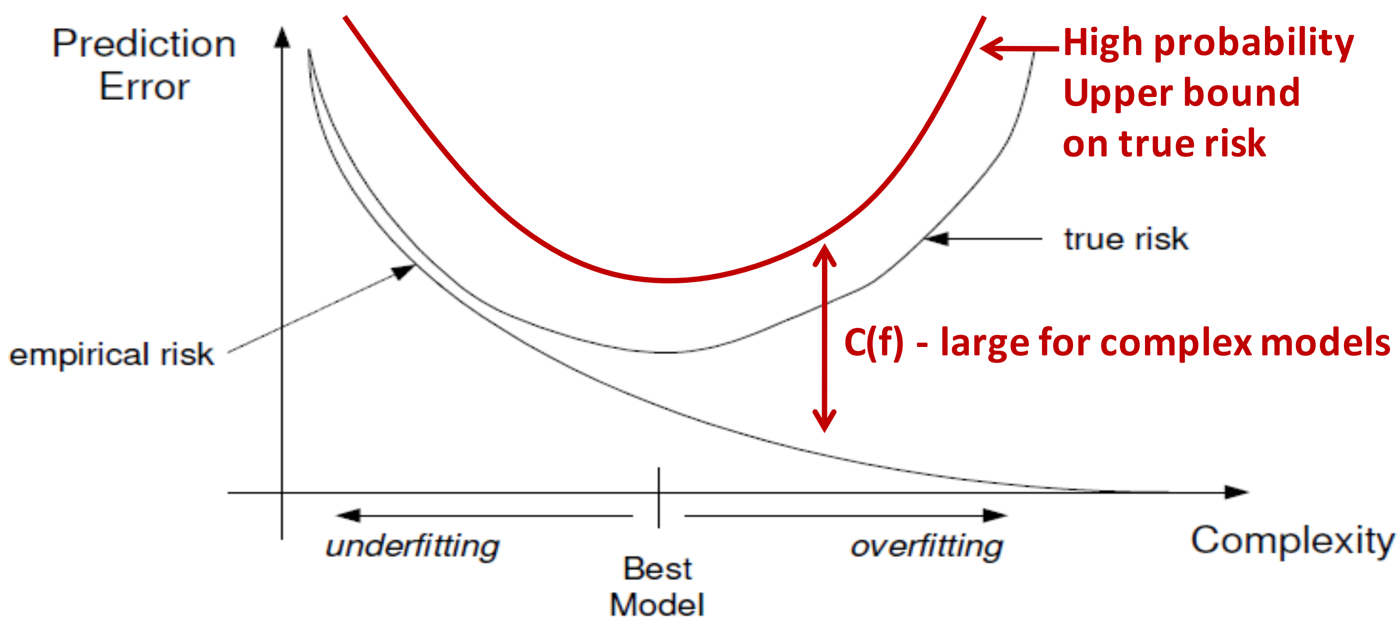
Suppose we have a bound, that with high probability:

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

Concentration bounds (later)

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

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



Risk Minimization

- OK, so we know how to estimate the “true risk” well, of an existing estimator e.g. empirical risk minimizer
- So now we can go back to solving the problem that empirical risk minimization might not be the right thing to do when the model complexity is high
  - i.e. it might overfit
  - with our great measures of "true risk", we might even get an indicator that hey it is overfitting
  - but what do we do with this information?
- We should not just estimate the true risk of an existing estimator, but our existing estimator should minimize the true risk!

Risk Minimization

- How do we improve empirical risk minimization with our newfound knowledge of how to better estimate true risk?

- Two-staged approach:
  - Given a model class, use better estimates of true risk to improve **empirical risk minimization**
    - Structural Risk Minimization
    - Regularize Empirical Risk with Model Complexity
      - Prior Information
      - Information-theoretic Criteria
    - We cannot use algorithmic risk estimates (e.g. cross-validation) because would be too expensive to train an estimator
  - Select model class (i.e."tuning parameters") using better true risk estimates
    - We CAN use algorithmic risk estimates (e.g. cross-validation) since only finitely many options to choose from

IMPROVING EMPIRICAL RISK MINIMIZATION

Structural Risk Minimization

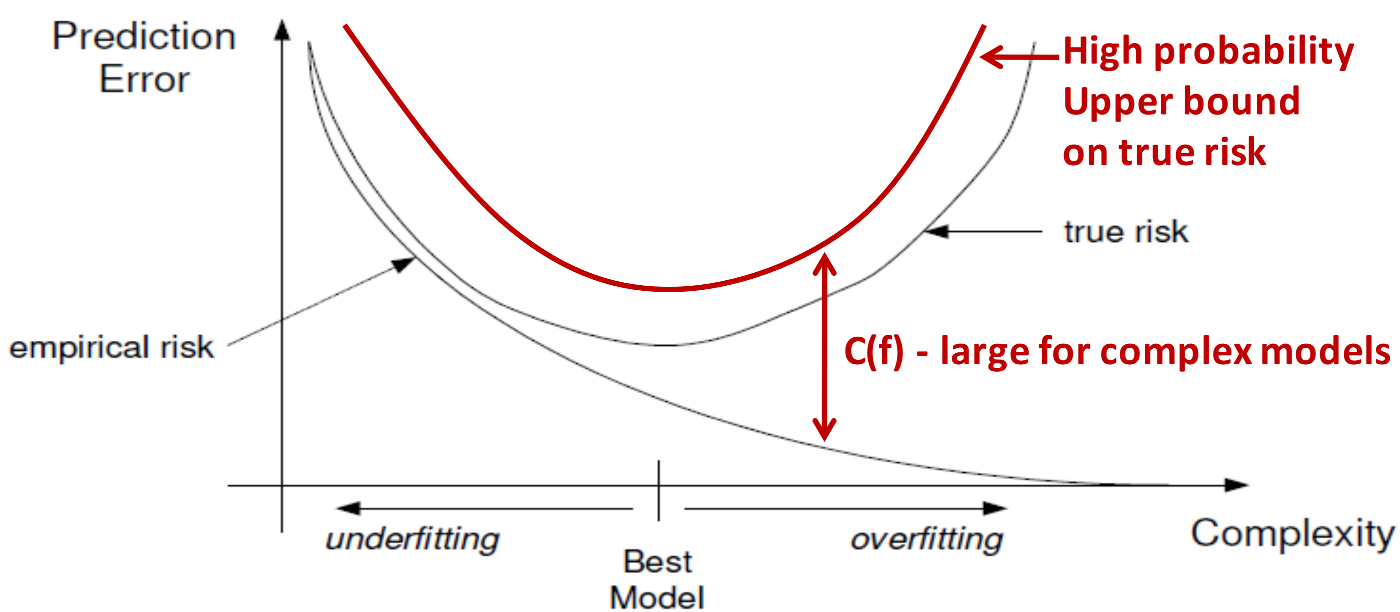
Penalize models using bound on **deviation of true and empirical risks**.

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

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)



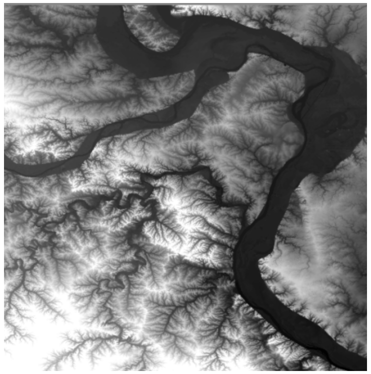
Structural Risk Minimization

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

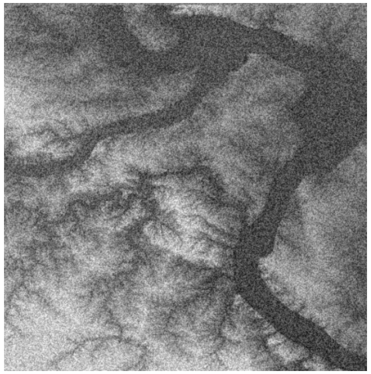
$$\widehat{f}_n = \arg\min_{f \in \mathcal{F}} \left\{ \widehat{R}_n(f) + \lambda C(f) \right\}$$

Choose by **model selection**!

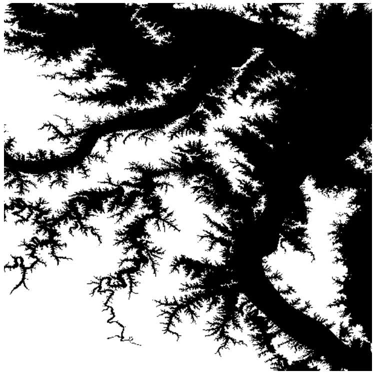
Problem: Identify flood plain from noisy satellite images



Noiseless image



Noisy image



True Flood plain
(elevation level > x)

Structural Risk Minimization

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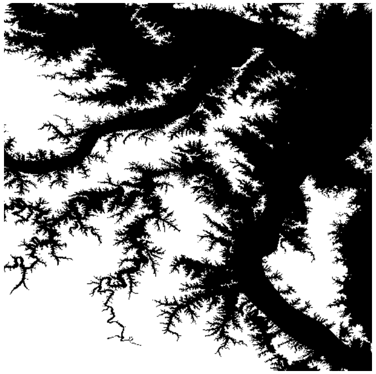

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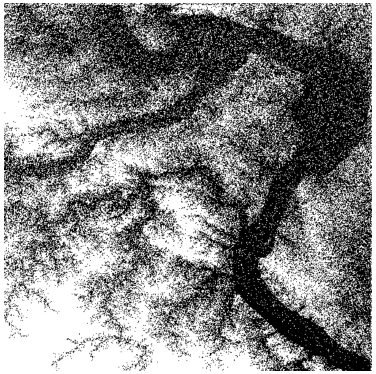
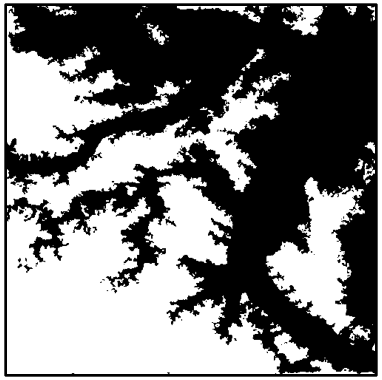
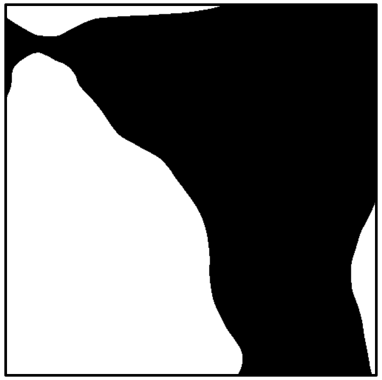
(elevation level > x)



Zero penalty

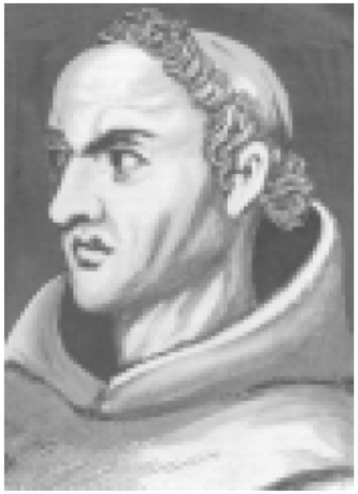


CV penalty



Theoretical penalty

Occam's Razor



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

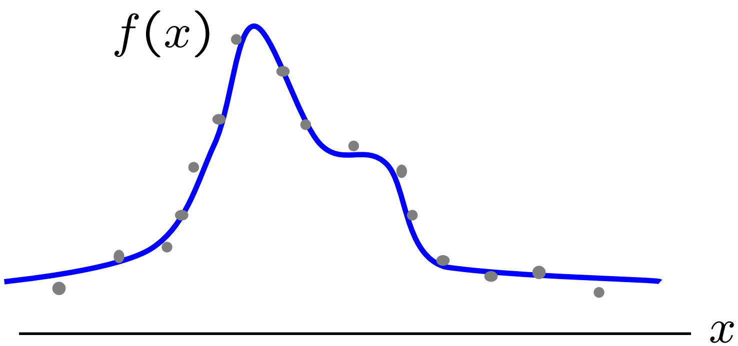
"One should not increase, beyond what is necessary, the number of entities required to explain anything."

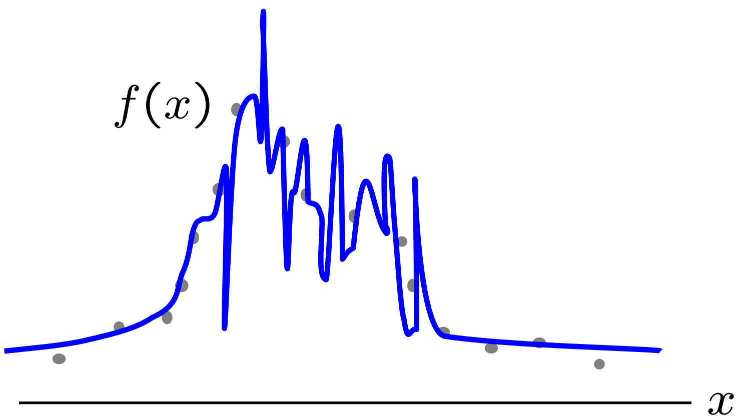
Alternatively, seek the simplest explanation.

Penalize complex models based on

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

Importance of Domain knowledge





Distribution of photon arrivals

Oil Spill Contamination

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? **Cross-validation**

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

MODEL SELECTION

Model Selection

- Model Classes with increasing complexity

- Regression with polynomials of order k = 0, 1, 2, …
  - Higher degree => Higher complexity
  - Question: How to select k?
- Regularization parameter lambda in previous estimators
  - Larger values of lambda => Lower complexity
  - Question: How to select lambda?

- The general setup:
  - Have a finite set of model classes (indexed by some "tuning parameter") with differing model complexities
  - Given any one model class, can use estimates of true risk to find optimal estimator
  - Model selection: find the optimal model class

Model Selection

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 lambda, pick estimator f_lambda using

- empirical risk minimization
- structural risk minimization
- complexity regularized risk minimization

Stage II: Pick that lambda for which f_lambda has least true risk estimated using

- cross-validation
- holdout
- information-theoretic risk estimates

A more theoretical understanding these two stages of the risk minimization story

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

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

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

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

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

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

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

Above is random due to samples in training data

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

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

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

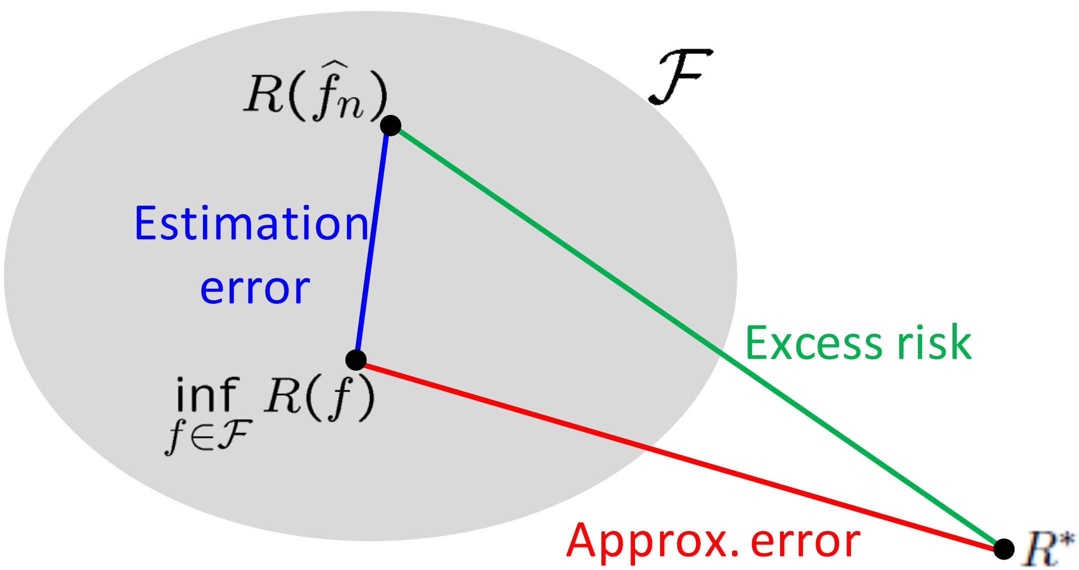
Behavior of True Risk

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

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

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

Due to restriction of model class

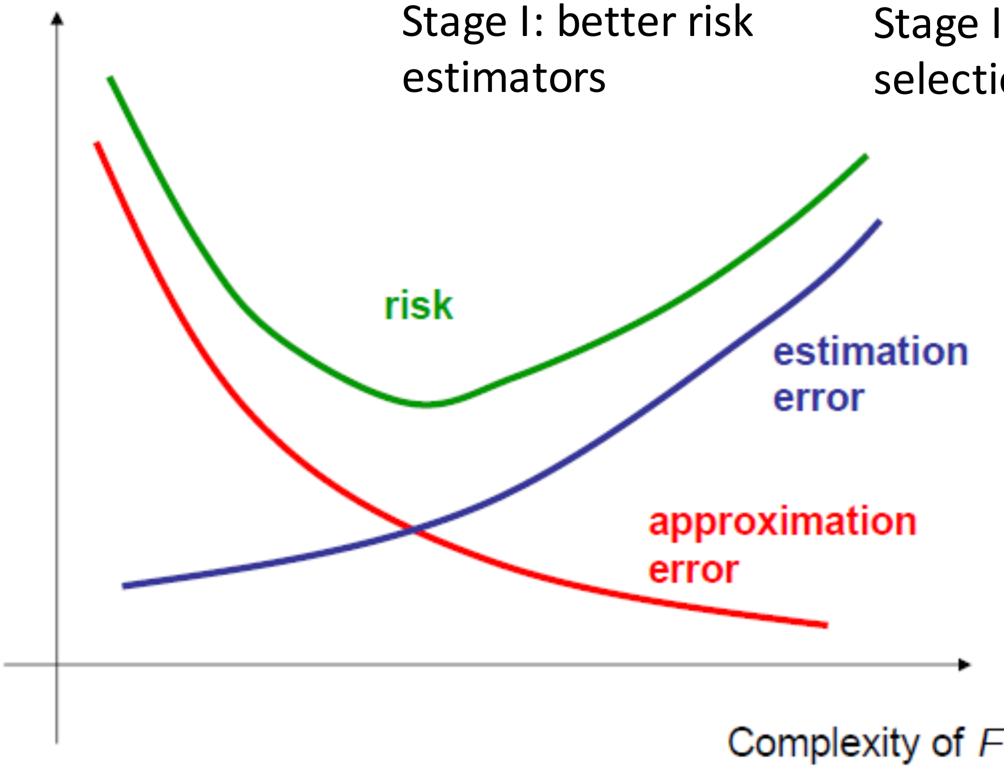


Behavior of True Risk

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

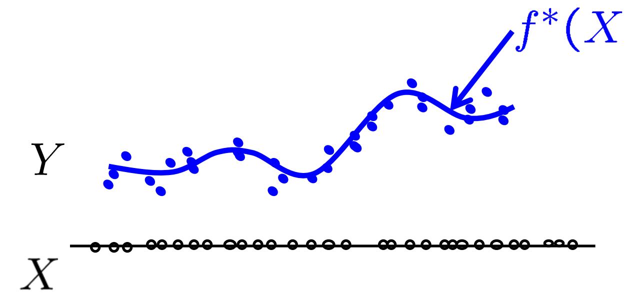
Stage I: better risk estimators

Stage II: model selection



Bias – Variance Tradeoff

Regression: $Y = f^*(X) + \epsilon \qquad \epsilon \sim \mathcal{N}(0, \sigma^2)$



$$R^* = \mathbb{E}_{XY}[(f^*(X) - Y)^2] = \mathbb{E}[\epsilon^2] = \sigma^2$$

Notice: Optimal predictor does not have zero error

$$\mathbb{E}_{D_n}[R(\widehat{f}_n)] = \mathbb{E}_{X,Y,D_n}[(\widehat{f}_n(X) - Y)^2]$$

D_n - training data of size n

$$\vdots$$

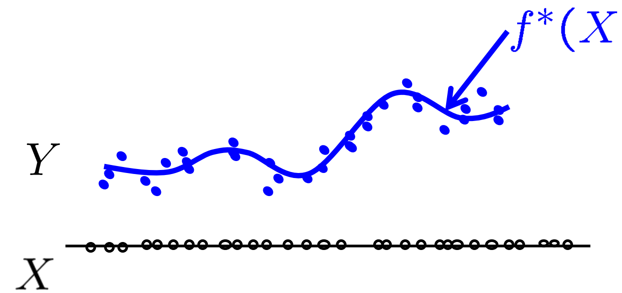
$$= \underbrace{\mathbb{E}_{X,Y,D_n}[(\widehat{f}_n(X) - \mathbb{E}_{D_n}[\widehat{f}_n(X)])^2]}_{\text{variance}} + \underbrace{\mathbb{E}_{X,Y}[(\mathbb{E}_{D_n}[\widehat{f}_n(X)] - f^*(X))^2]}_{\text{bias}^\wedge 2} + \underbrace{\sigma^2}_{\text{Noise var}}$$

Excess Risk = $\mathbb{E}_{D_n}[R(\widehat{f}_n)] - R^*$ = variance + bias^2

Random component ≡ est err

≡ approx err

Bias – Variance Tradeoff: Derivation



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$$\mathbb{E}_{D_n}[R(\widehat{f}_n)] = \mathbb{E}_{X,Y,D_n}[(\widehat{f}_n(X) - Y)^2]$$

D_n - training data of size n

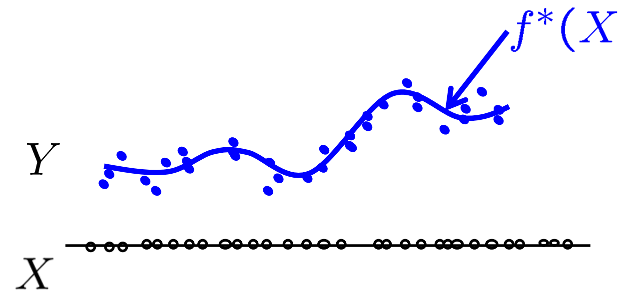
$$= \mathbb{E}_{X,Y,D_n}\left[(\widehat{f}_n(X) - \mathbb{E}_{D_n}[\widehat{f}_n(X)] + \mathbb{E}_{D_n}[\widehat{f}_n(X)] - Y)^2\right]$$

$$= \mathbb{E}_{X,Y,D_n}\Big[(\widehat{f}_n(X) - \mathbb{E}_{D_n}[\widehat{f}_n(X)])^2 + (\mathbb{E}_{D_n}[\widehat{f}_n(X)] - Y)^2$$
$$+2(\widehat{f}_n(X) - \mathbb{E}_{D_n}[\widehat{f}_n(X)])(\mathbb{E}_{D_n}[\widehat{f}_n(X)] - Y)\Big]$$

$$= \mathbb{E}_{X,Y,D_n}\left[(\widehat{f}_n(X) - \mathbb{E}_{D_n}[\widehat{f}_n(X)])^2\right] + \mathbb{E}_{X,Y,D_n}\left[(\mathbb{E}_{D_n}[\widehat{f}_n(X)] - Y)^2\right]$$
$$+\mathbb{E}_{X,Y}\left[2(\underbrace{\cancel{\mathbb{E}_{D_n}[\widehat{f}_n(X)] - \mathbb{E}_{D_n}[\widehat{f}_n(X)]}}_{\mathbf{0}})(\mathbb{E}_{D_n}[\widehat{f}_n(X)] - Y)\right]$$

Bias – Variance Tradeoff: Derivation

Regression: $Y = f^*(X) + \epsilon \qquad \epsilon \sim \mathcal{N}(0, \sigma^2)$



$$R^* = \mathbb{E}_{XY}[(f^*(X) - Y)^2] = \mathbb{E}[\epsilon^2] = \sigma^2$$

Notice: Optimal predictor does not have zero error

$$\mathbb{E}_{D_n}[R(\widehat{f}_n)] = \mathbb{E}_{X,Y,D_n}[(\widehat{f}_n(X) - Y)^2]$$

D_n - training data of size n

$$= \underbrace{\mathbb{E}_{X,Y,D_n}\left[(\widehat{f}_n(X) - \mathbb{E}_{D_n}[\widehat{f}_n(X)])^2\right]} + \mathbb{E}_{X,Y,D_n}\left[(\mathbb{E}_{D_n}[\widehat{f}_n(X)] - Y)^2\right]$$

variance – how much does the predictor vary about its mean for different training datasets

Now, lets look at the second term:

$$\mathbb{E}_{X,Y,D_n}\left[(\mathbb{E}_{D_n}[\widehat{f}_n(X)] - Y)^2\right] = \mathbb{E}_{X,Y}\left[(\mathbb{E}_{D_n}[\widehat{f}_n(X)] - Y)^2\right]$$

Note: this term doesn't depend on D_n

Bias – Variance Tradeoff: Derivation

$$\begin{aligned}
\mathbb{E}_{X,Y}\left[(\mathbb{E}_{D_n}[\widehat{f}_n(X)] - Y)^2\right] &= \mathbb{E}_{X,Y}\left[(\mathbb{E}_{D_n}[\widehat{f}_n(X)] - f^*(X) - \epsilon)^2\right] \\
&= \mathbb{E}_{X,Y}\Big[(\mathbb{E}_{D_n}[\widehat{f}_n(X)] - f^*(X))^2 + \epsilon^2 \\
&\qquad -2\epsilon(\mathbb{E}_{D_n}[\widehat{f}_n(X)] - f^*(X))\Big] \\
&= \mathbb{E}_{X,Y}\left[(\mathbb{E}_{D_n}[\widehat{f}_n(X)] - f^*(X))^2\right] + \mathbb{E}_{X,Y}\left[\epsilon^2\right] \\
&\qquad \cancel{-2\mathbb{E}_{X,Y}\left[\epsilon(\mathbb{E}_{D_n}[\widehat{f}_n(X)] - f^*(X))\right]}
\end{aligned}$$

0 since noise is independent and zero mean

$$= \underbrace{\mathbb{E}_{X,Y}\left[(\mathbb{E}_{D_n}[\widehat{f}_n(X)] - f^*(X))^2\right]}_{\text{bias}^2} + \underbrace{\mathbb{E}_{X,Y}\left[\epsilon^2\right]}_{\text{noise variance}}$$

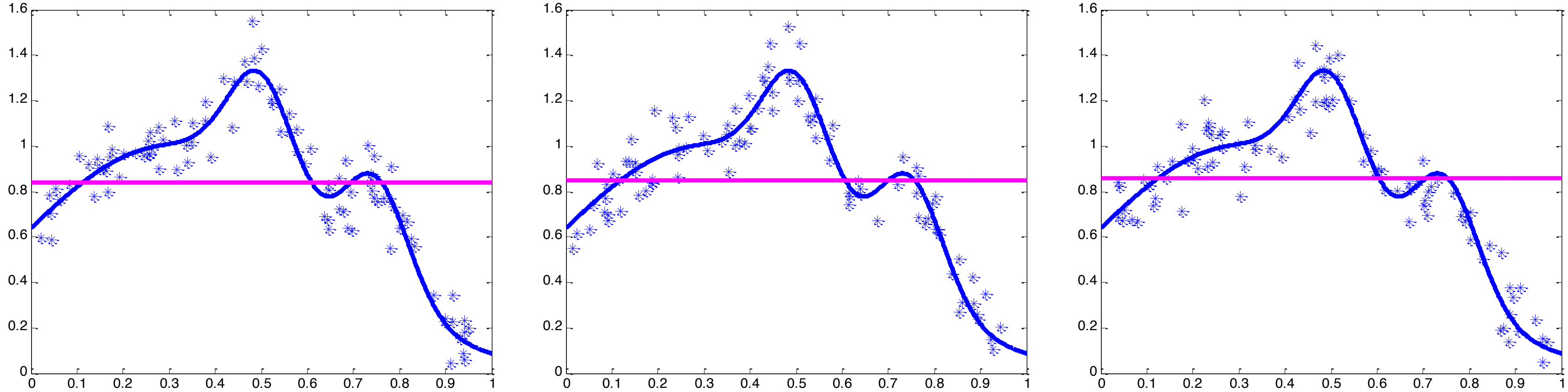
bias^2 – how much does the mean of the predictor differ from the optimal predictor

noise variance

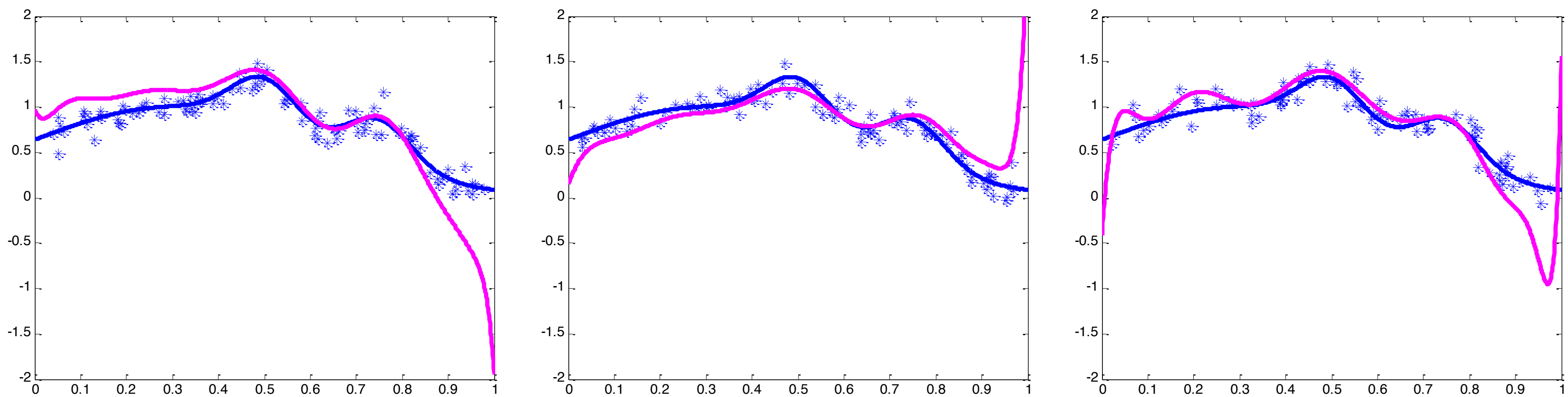
Bias – Variance Tradeoff

3 Independent training datasets

Large bias, Small variance – poor approximation but robust/stable



Small bias, Large variance – good approximation but unstable



Summary

True and Empirical Risk

Over-fitting

Model Selection, Estimating Generalization Error

- Hold-out, K-fold cross-validation
- Structural Risk Minimization
- Complexity Regularization
- Information Criteria – AIC, BIC

- Approx err vs Estimation err, Bias vs Variance tradeoff