Practical Issues in Machine Learning
Overfitting and 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 $\mathbb{E}[(f(X) - Y)^2]$

Also known as "Generalization Error" – performance on a random test point (X,Y)

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Empirical Risk: Performance on training data

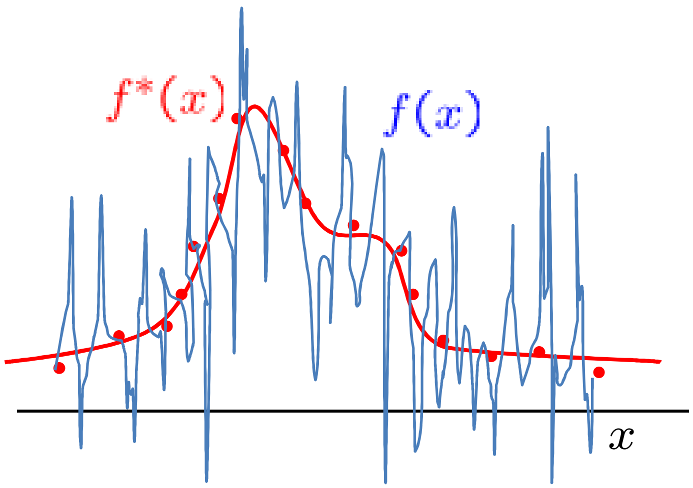
Classification – Proportion of misclassified examples $\frac{1}{n}\sum_{i=1}^{n} 1_{f(X_i) \neq Y_i}$

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

Overfitting

Is the following predictor a good one?

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



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 !

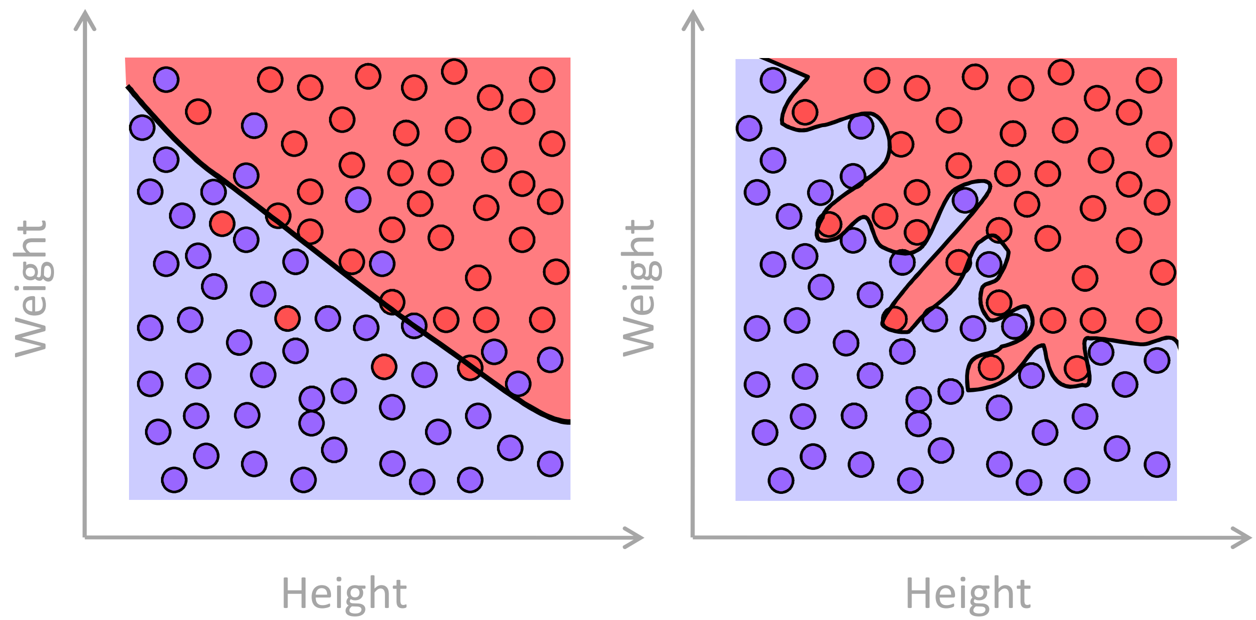
Overfitting

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

Examples: Classification (0-NN classifier, decision tree with one sample/leaf)

Football player ?

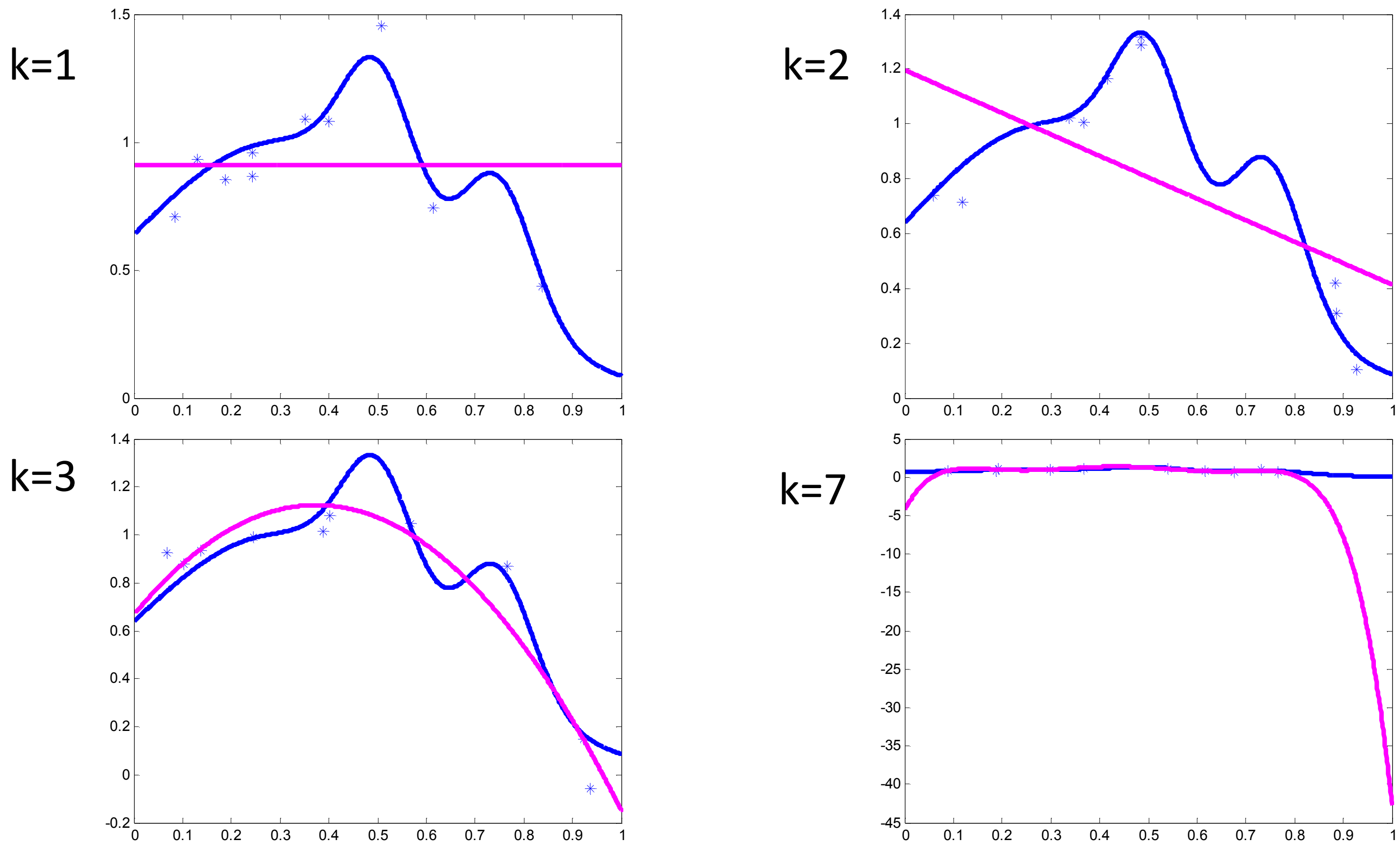
- No
- Yes



Overfitting

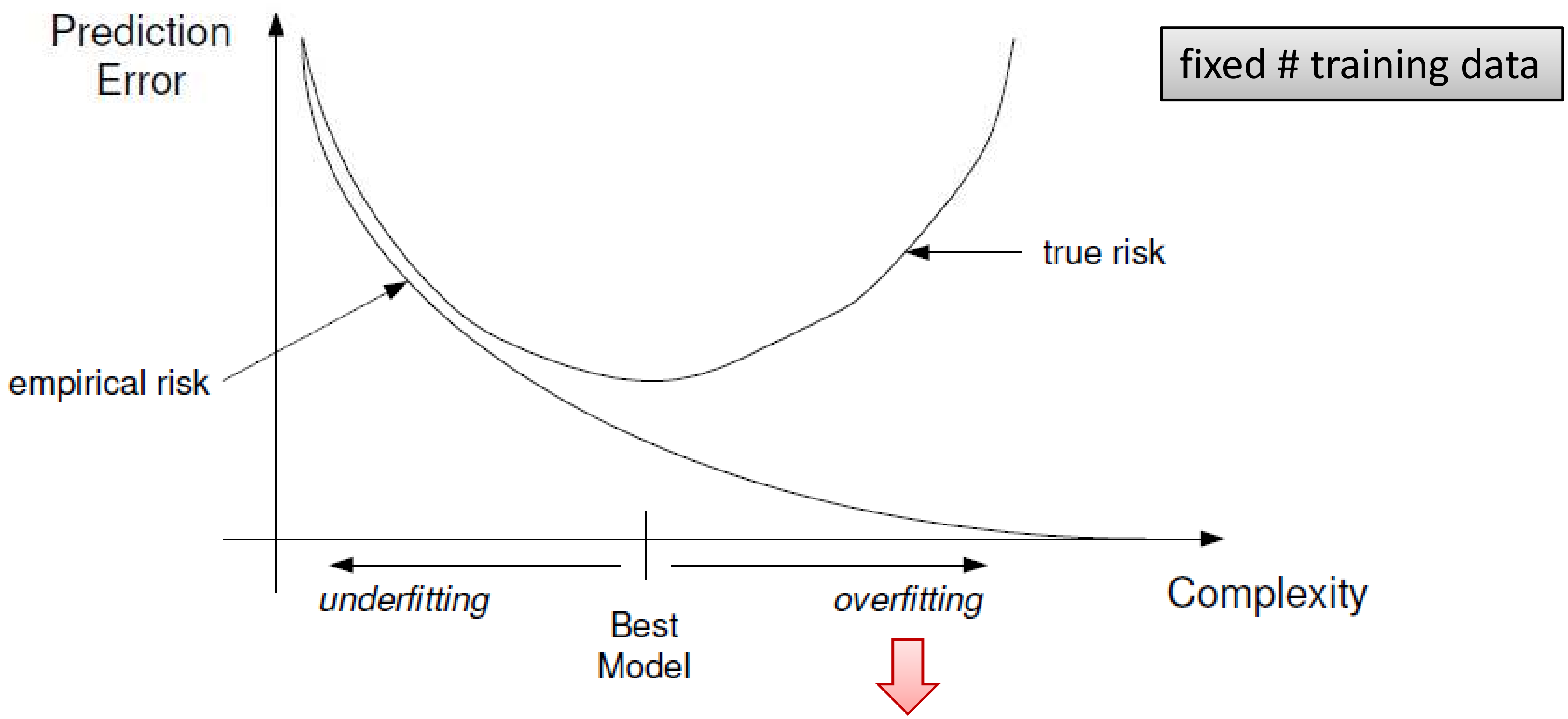
If we allow very complicated predictors, we could overfit the training data.

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



Effect of Model Complexity

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



Empirical risk is no longer a good indicator of true risk

Behavior of True Risk

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

Excess Risk $E\left[R(\widehat{f}_n)\right] - R^*$

wrt the distribution of training data

- Why is the risk of $\widehat{f}_n$ a random quantity?

$$R(\widehat{f}_n) = P_{XY}(\widehat{f}_n(X) \neq Y)$$

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

$\widehat{f}_n$ depends on random training dataset

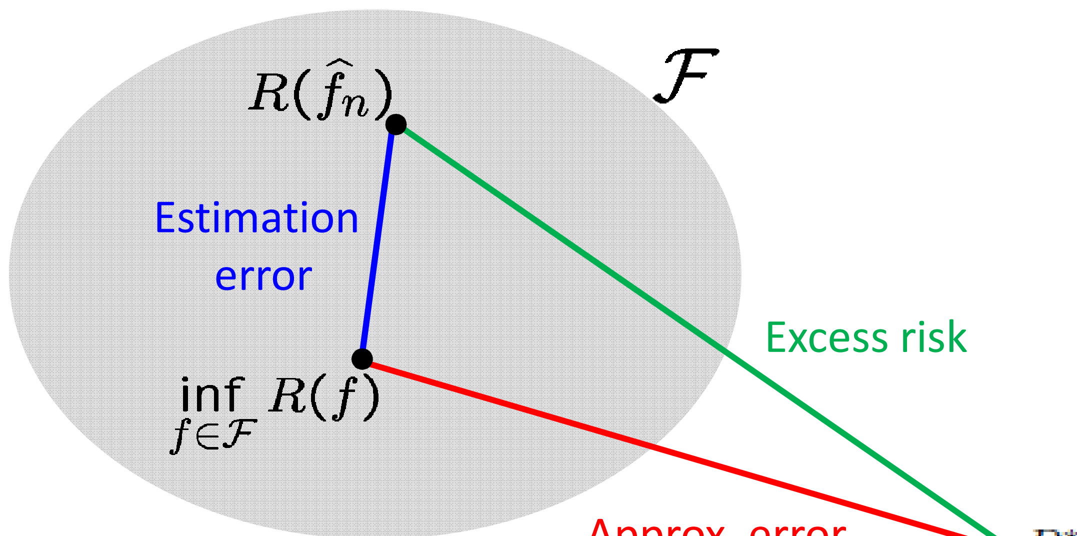
Behavior of True Risk

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

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

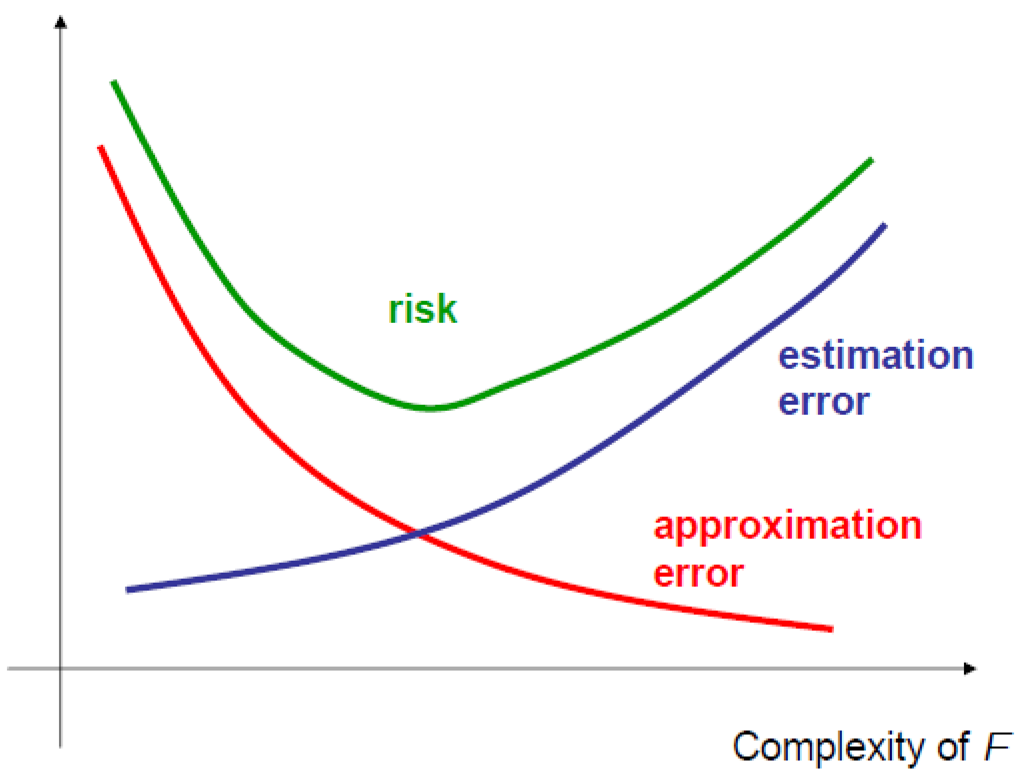
finite sample size + noise ← Due to randomness of training data

Due to restriction of model class



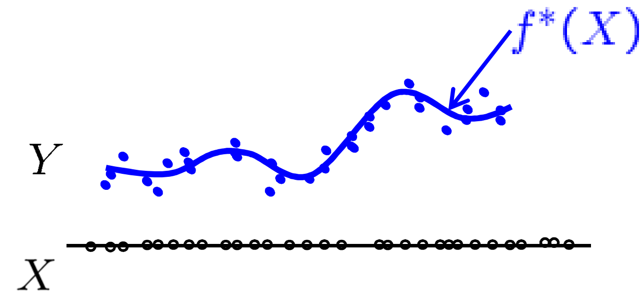
Behavior of True Risk

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



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

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

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

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

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

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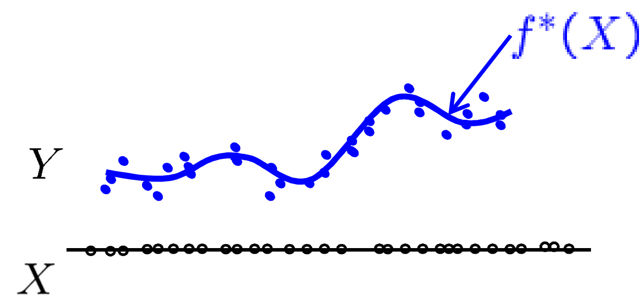

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Notice: Optimal predictor does not have zero error

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

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

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

Now, lets look at the second term:

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

<u>Note:</u> this term doesn't depend on D

Bias – Variance Tradeoff

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

0 since noise is independent and zero mean

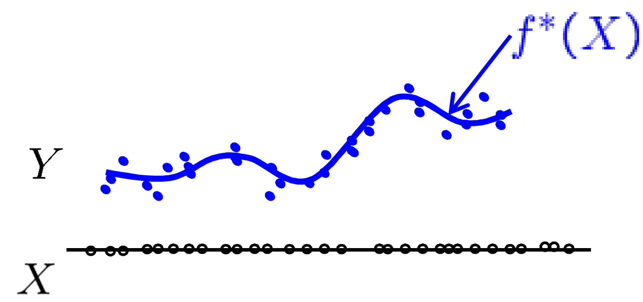
$$= \underbrace{\mathbb{E}_{X,Y}\left[(\mathbb{E}_D[\widehat{f}_n(X)] - f^*(X))^2\right]}_{\text{bias}^2} + \underbrace{\mathbb{E}_{X,Y}\left[\epsilon^2\right]}_{\text{noise variance}}$$

bias^2 – how much does the predictor on average differ from the optimal predictor

noise variance

Bias – Variance Tradeoff

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



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Notice: Optimal predictor does not have zero error

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

$$\vdots$$

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

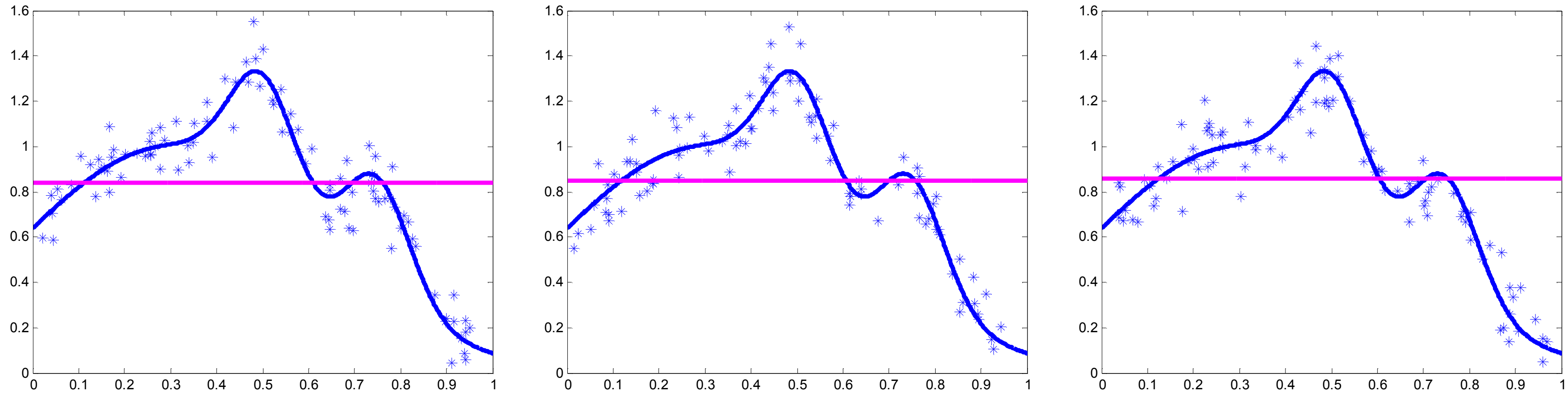
Excess Risk = $\mathbb{E}_D[R(\widehat{f}_n)] - R^*$ = variance + bias^2

Random component $\equiv$ est err $\qquad \equiv$ approx err

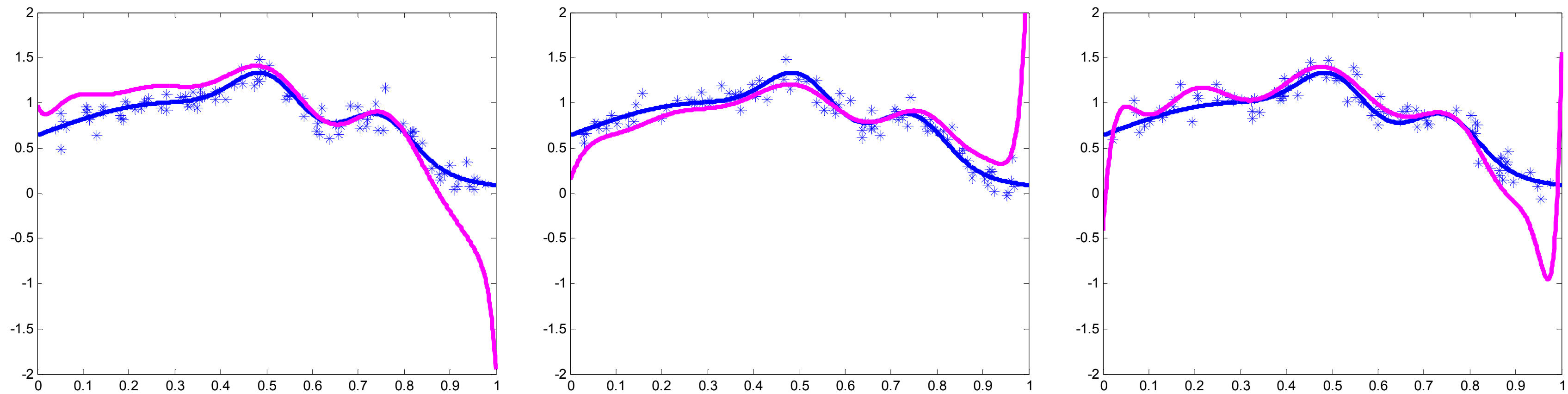
Bias – Variance Tradeoff

3 Independent training datasets

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



Small bias, Large variance – good approximation but instable



Examples of Model Spaces

Model Spaces with increasing complexity:

- Nearest-Neighbor classifiers with varying neighborhood sizes k = 1,2,3,…
  Small neighborhood => Higher complexity
- Decision Trees with depth k or with k leaves
  Higher depth/ More # leaves => Higher complexity
- Regression with polynomials of order k = 0, 1, 2, …
  Higher degree => Higher complexity
- Kernel Regression with bandwidth h
  Small bandwidth => Higher complexity

How can we select the right complexity model ?

Model Selection

Setup:

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

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

We can select the right complexity model in a data-driven/adaptive way:

- ❑ Cross-validation
- ❑ Method of Sieves
- ❑ Structural Risk Minimization
- ❑ Complexity Regularization
- ❑ *Information Criteria* - Minimum Description Length, AIC, BIC

Hold-out method

We would like to pick the model that has smallest generalization error.

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

NOT test Data !!

2) Use D_T for training a predictor from each model class:

$$\widehat{f}_\lambda = \arg\min_{f \in \mathcal{F}_\lambda} \widehat{R}_T(f)$$

Evaluated on training dataset D_T

Hold-out method

3) Use D_V to select the model class which has smallest empirical error on D_V

$$\widehat{\lambda} = \arg\min_{\lambda \in \Lambda} \widehat{R}_V(\widehat{f}_\lambda)$$

Evaluated on validation dataset D_V

4) Hold-out predictor

$$\widehat{f} = \widehat{f}_{\widehat{\lambda}}$$

Intuition: Small error on one set of data will not imply small error on a randomly sub-sampled second set of data

Ensures method is "stable"

Hold-out method

Drawbacks:

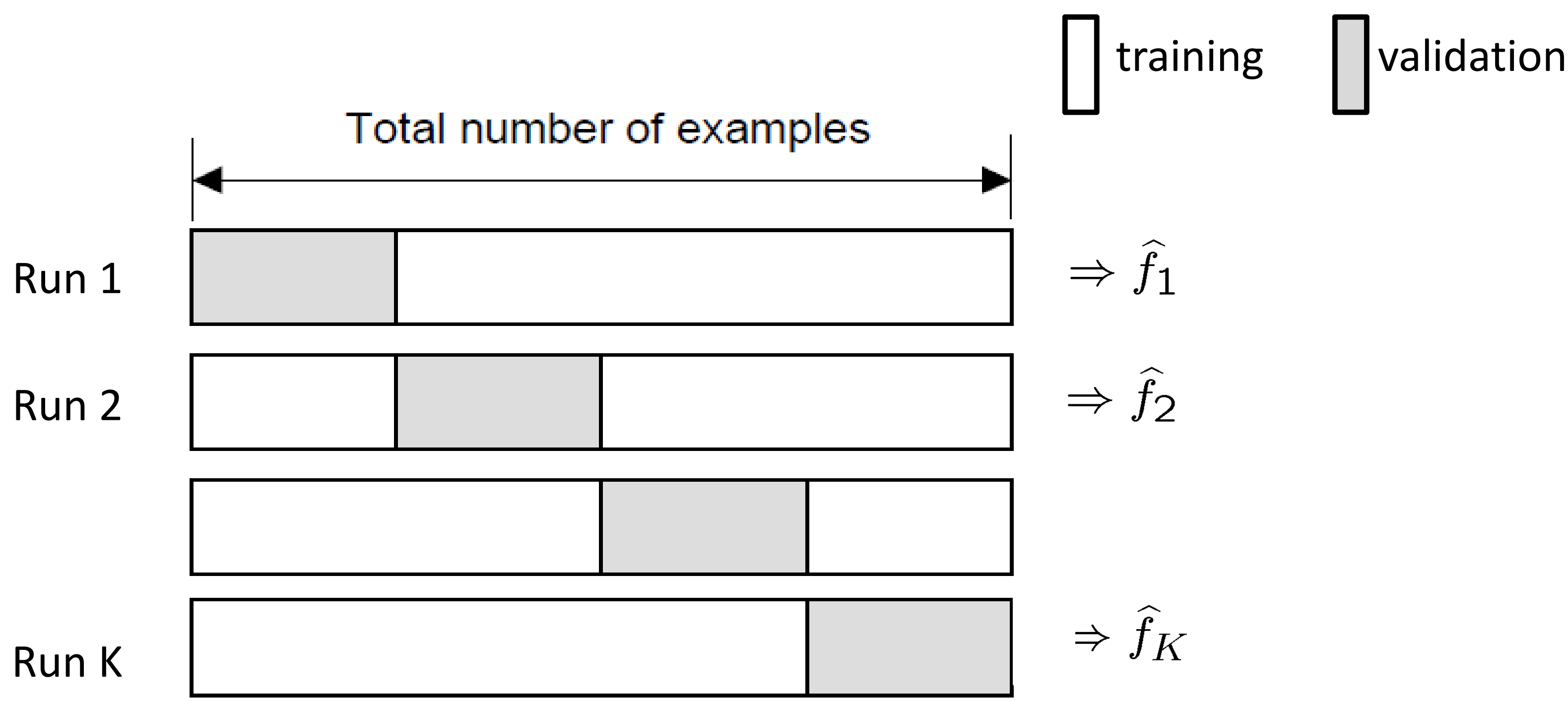
- May not have enough data to afford setting one subset aside for getting a sense of generalization abilities
- Validation error may be misleading (bad estimate of generalization error) if we get an "unfortunate" split

Limitations of hold-out can be overcome by a family of random sub-sampling methods at the expense of more computation.

Cross-validation

K-fold cross-validation

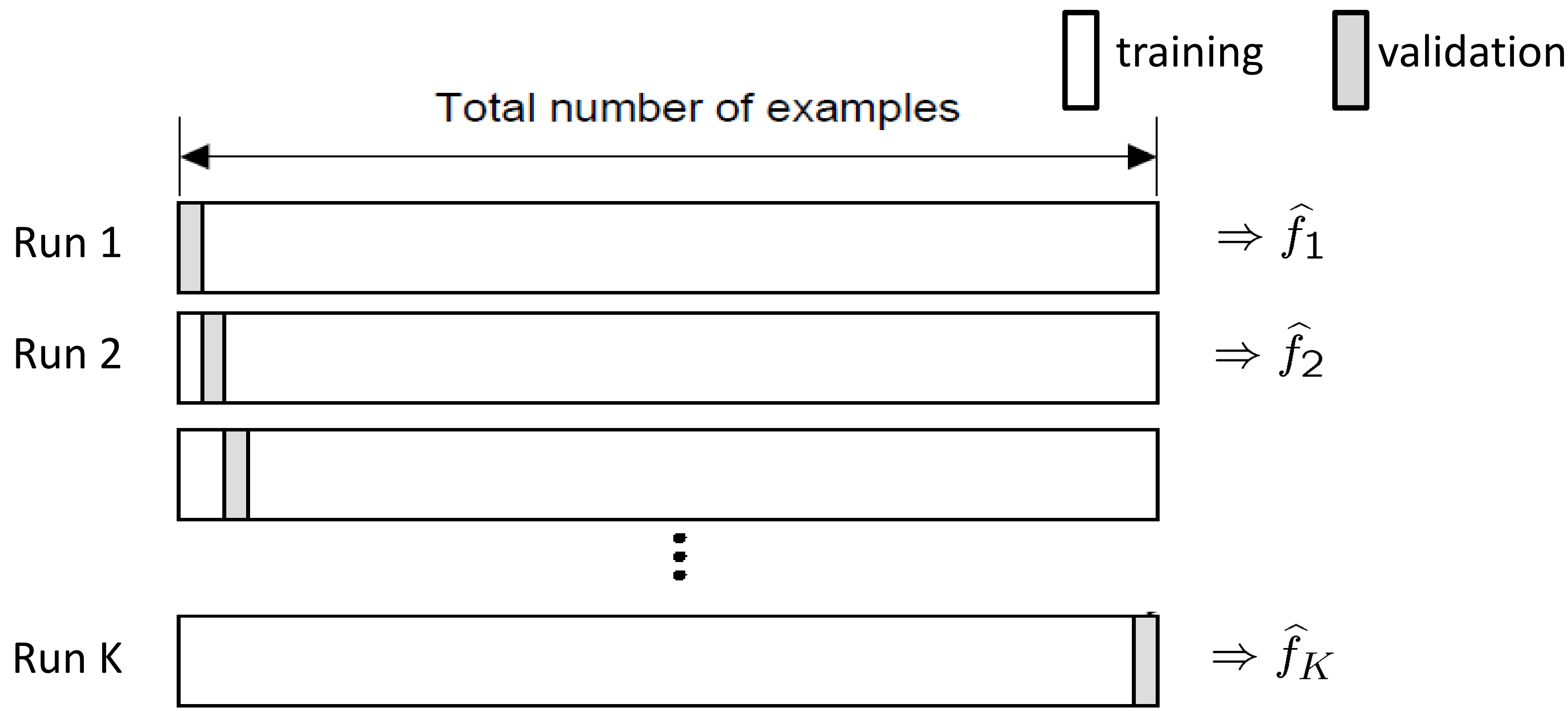
Create K-fold partition of the dataset.
Form K hold-out predictors, each time using one partition as validation and rest K-1 as training datasets.
Final predictor is average/majority vote over the K hold-out estimates.



Cross-validation

<u>Leave-one-out (LOO) cross-validation</u>

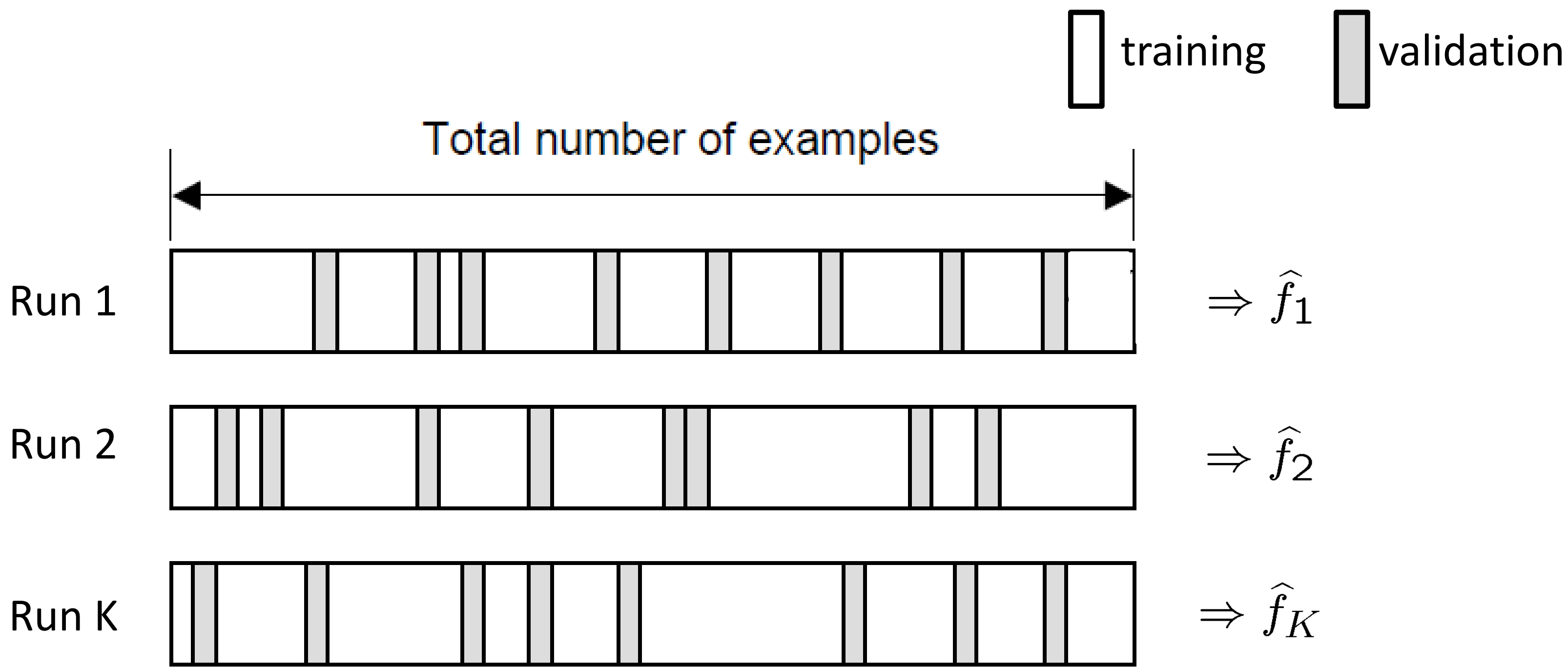
Special case of K-fold with K=n partitions
Equivalently, train on n-1 samples and validate on only one sample per run for n runs



Cross-validation

Random subsampling

Randomly subsample a fixed fraction αn (0< α <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 generalization error

Generalization error $\mathbb{E}_D[R(\widehat{f}_n)]$

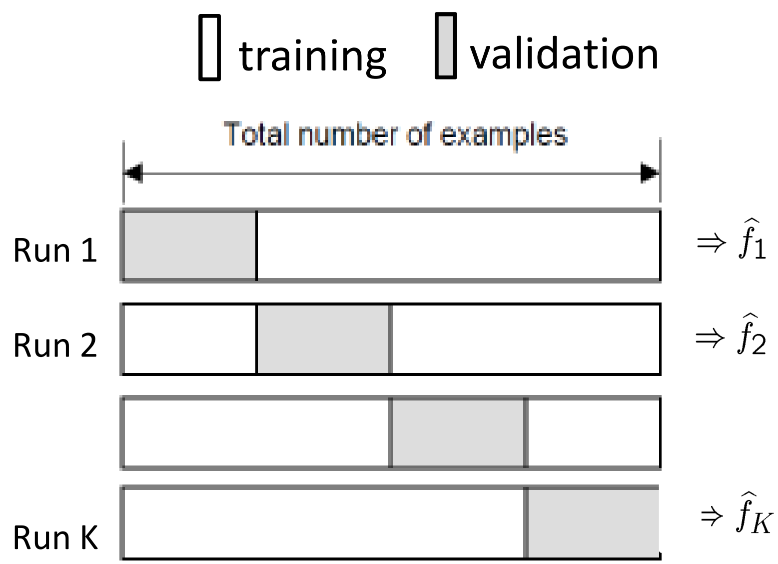
Hold-out ≡ 1-fold: Error estimate = $\widehat{R}_V(\widehat{f}_T)$

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
  - 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
  - The bias of the error estimate will be large

In practice, the choice of the number of folds depends on the size of the dataset:

For large datasets, even 3-Fold Cross Validation will be quite accurate
For very sparse datasets, we may have to use leave-one-out in order to train on as many examples as possible

- A common choice is K=10 and $\alpha = 0.1$

Occam’s Razor

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

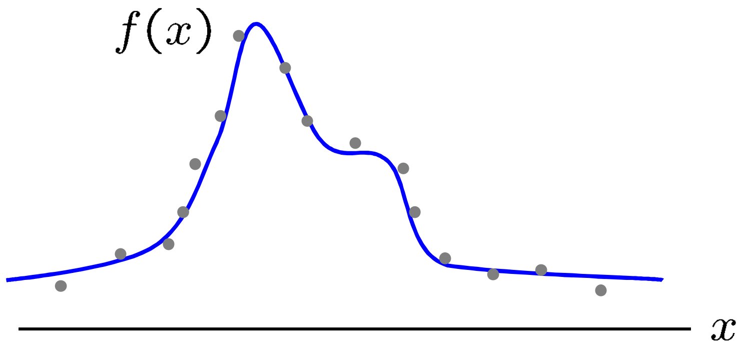
“One should not increase, beyond what is necessary, the number of entities required to explain anything.”

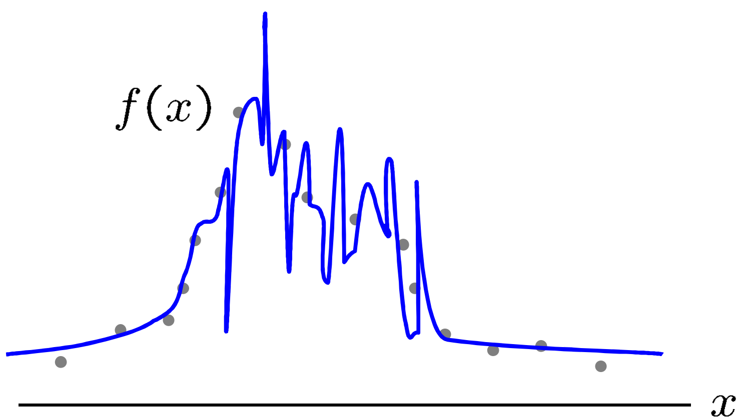
Alternatively, seek the simplest explanation.

Penalize complex models based on

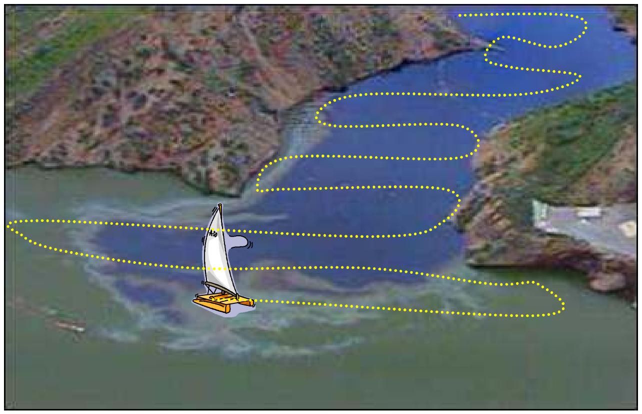
- Prior information (bias)
- Information Criterion (MDL, AIC, BIC)

Importance of Domain knowledge





Distribution of photon arrivals



Oil Spill Contamination

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

Method of Sieves

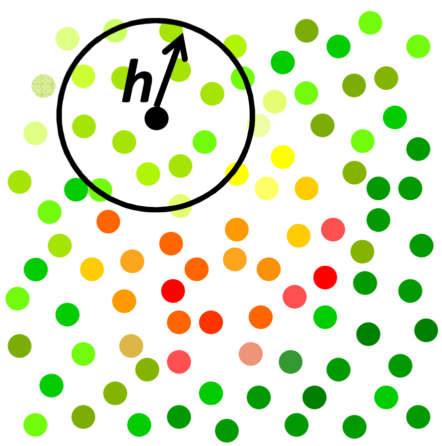
Consider a sequence of models whose complexity grows with # training data, n

$$\mathcal{F}_1 \prec \mathcal{F}_2 \prec \ldots \mathcal{F}_n \prec \ldots$$

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

Why does optimal complexity depend on # training data?

Consider kernel regression in d-dimensions: complexity ≡ bandwidth h



Large h – average more data points, reduce noise

Lower variance $\propto \frac{1}{nh^d}$ = # pts in h-ball

Small h – less smoothing, more accurate fit

Lower bias $\propto h^{\alpha}$ → Smoothness of target function

Method of Sieves

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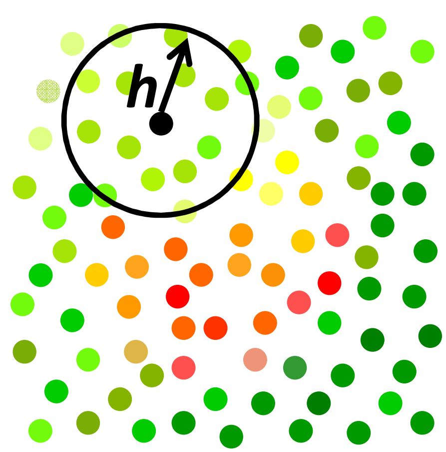


Bias-variance tradeoff:

Bias^2 + Variance $\propto h^{2\alpha} + \frac{1}{nh^d}$

If smoothness α is known, we can choose bandwidth h as: $h \asymp n^{-\frac{2\alpha}{2\alpha+d}}$

How to choose scaling constant? **Cross-validation**

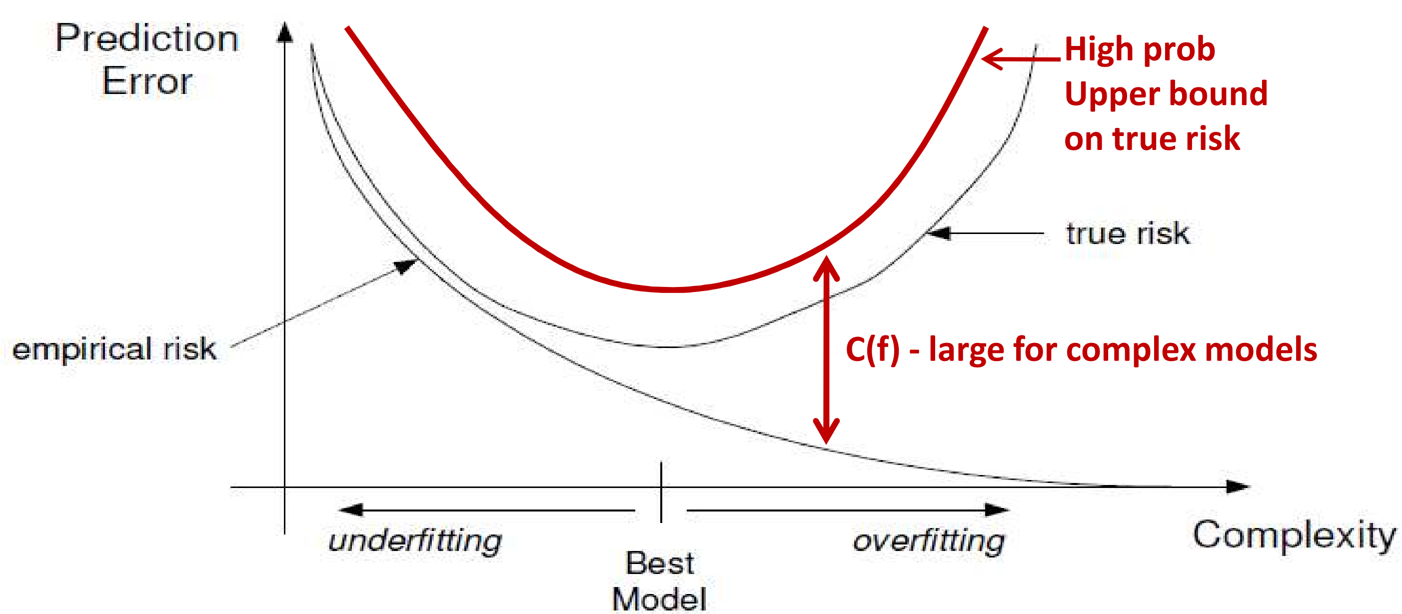
Structural Risk Minimization

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)



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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)

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

$$\leq \min_{f \in \mathcal{F}} \{ R(f) + 2C(f) \}$$

$$R(\widehat{f}_n) - R^* \leq \underbrace{\min_{f \in \mathcal{F}} \{ R(f) - R^*}_{\text{approx err}} + \underbrace{2C(f)}_{\text{est err}} \}$$

Structural Risk Minimization

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

Bound on deviation from true risk

How does structural risk minimization help in kernel regression?

Let $C(f) \propto \frac{1}{nh^d} \qquad \forall f \in \mathcal{F}_h$

With high prob. $R(\widehat{f}_n) - R^* \leq \min_{f \in \mathcal{F}} \{R(f) - R^* + 2C(f)\}$

$$\leq \min_h \min_{f \in \mathcal{F}_h} \{R(f) - R^* + 2C(f)\}$$

$$\propto \min_h \left\{ h^{2\alpha} + \frac{1}{nh^d} \right\}$$

Error automatically corresponds to best *h*

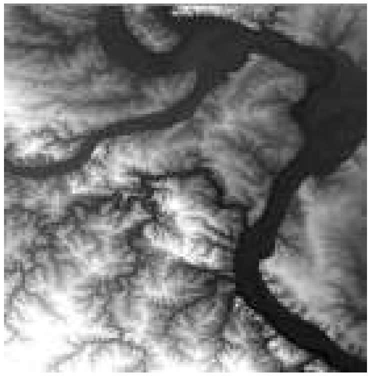
Structural Risk Minimization

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

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

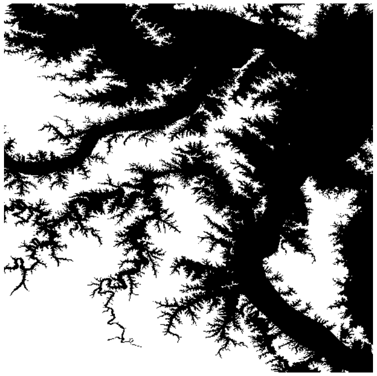
Choose by cross-validation!

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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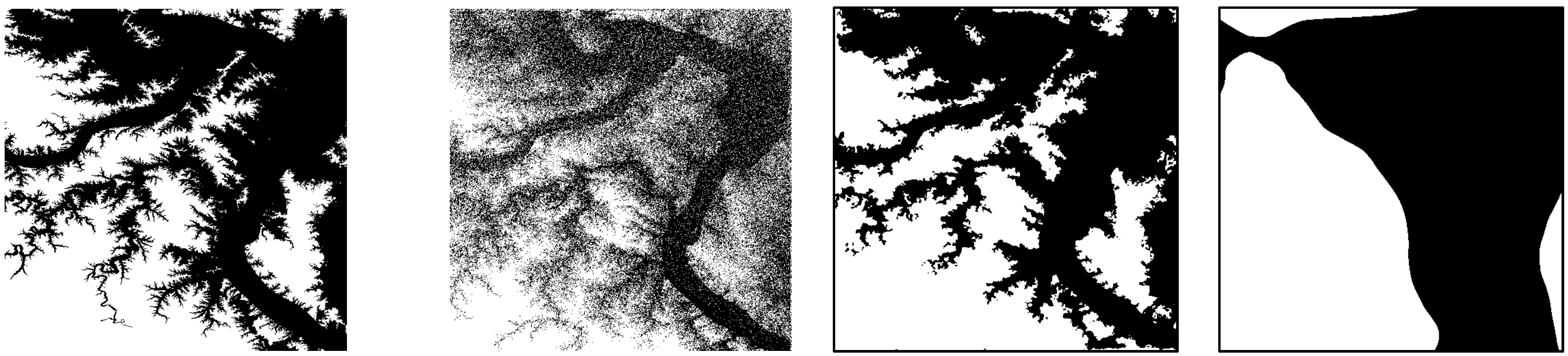


True Flood plain (elevation level > x) | Zero penalty | CV penalty | Theoretical penalty

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* ≡ $e^{-C(f)}$

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

ERM (empirical risk minimization) over a restricted class *F*, e.g. linear classifiers,
≡ 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

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

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

Penalize models based on some norm of regression coefficients

How to choose tuning parameter λ? **Cross-validation**

Information Criteria

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

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

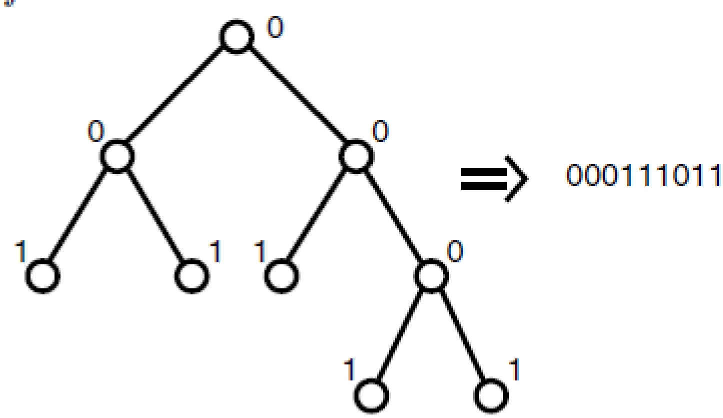
bits needed to describe f
(description length)

MDL (Minimum Description Length)

Example: Binary Decision trees $\mathcal{F}_k^T = \{\text{tree classifiers with } k \text{ leafs}\}$

$\mathcal{F}^T = \bigcup_{k \geq 1} \mathcal{F}_k^T$ prefix encode each element f of $\mathcal{F}^T$

$$C(f) = 3k - 1 \text{ bits}$$



k leaves => 2k – 1 nodes

2k – 1 bits to encode tree structure
+ k bits to encode label of each leaf (0/1)

5 leaves => 9 bits to encode structure

Information Criteria

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)

MDL (Minimum Description Length)

Other Information Criteria:

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

Summary

True and Empirical Risk

Over-fitting

Approx err vs Estimation err, Bias vs Variance tradeoff

Model Selection

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