Predictive Learning from Data

LECTURE SET 4

Statistical Learning Theory

(VC-theory)

Cherkassky, Vladimir, and Filip M. Mulier. *Learning from data: concepts, theory, and methods*. John Wiley & Sons, 2007.

Source: Dr. Vladimir Cherkassky (revised by Dr. Hsiang-Han Chen)

OUTLINE

- Objectives
- Inductive learning problem setting
- Statistical Learning Theory
- Applications
- Measuring the VC-dimension
- Summary and discussion

Motivation + Objectives

- Statistical Learning Theory (STL), also known as Vapnik-Chervonenkis (VC) Theory.
- One of the best theory for flexible statistical estimation with finite samples.
- STL adopts the goal of system imitation, rather than system identification.
- ***Goal:*** math theory for STL
- Three aspects of scientific theory: conceptual, technical, practical

Keep-It-Direct Principle

- The goal of learning is generalization rather than estimation of true function (system identification)

$$\int Loss(y, f(\mathbf{x},w))\, dP(\mathbf{x},y) \to min$$

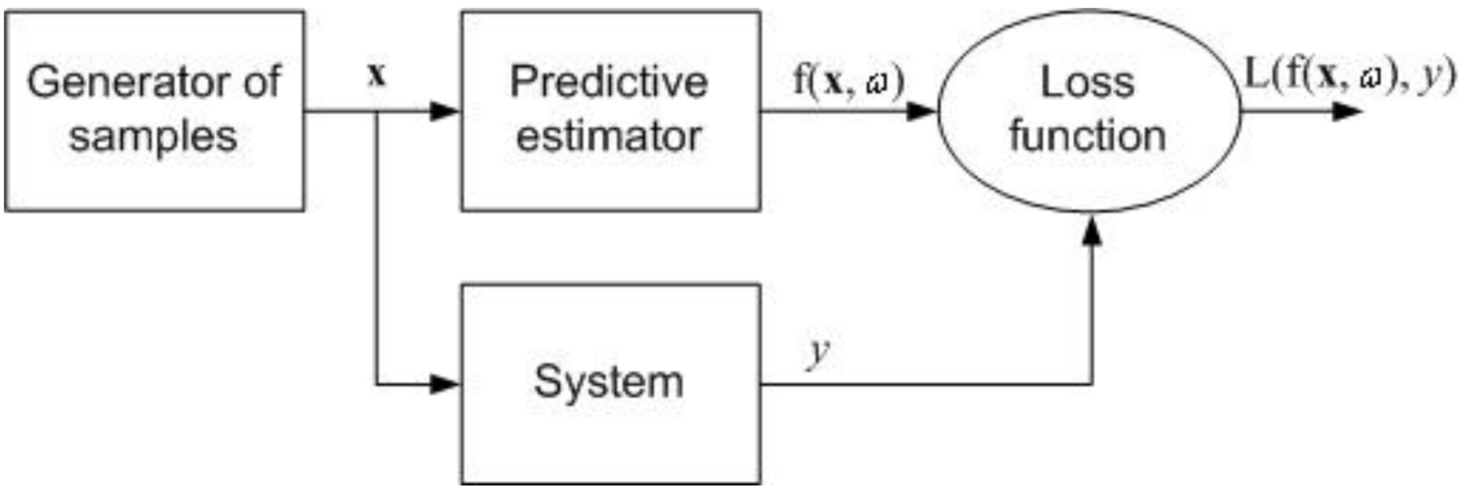
- **Keep-It-Direct Principle** (Vapnik, 1995)

  Do not solve an estimation problem of interest by solving a more general (harder) problem as an intermediate step
- Good predictive model reflects certain properties of unknown distribution $P(\mathbf{x},y)$
- Since model estimation with finite data is ill-posed, one should never try to solve a more general problem than required by a given application

  → Importance of formalizing application requirements as a predictive learning problem.

Inductive Learning Setting

- The learning machine observes samples ($\mathbf{x}$,y), and returns an estimated response $\hat{y} = f(\mathbf{x}, w)$
- Two modes of inference: identification vs imitation
- Risk $\int Loss(y, f(\mathbf{x},w))\, dP(\mathbf{x},y) \rightarrow min$



The Problem of Inductive Learning

- *Given:* finite training samples $\mathbf{Z}=\{(\mathbf{x}_i, y_i), i=1,2,\ldots n\}$ choose from a given set of functions $f(\mathbf{x}, \mathbf{w})$ the one that *approximates best* the true output. (in the sense of risk minimization)

Concepts and Terminology

- approximating functions $f(\mathbf{x}, \mathbf{w})$
- (non-negative) loss function $L(f(\mathbf{x}, \mathbf{w}),\mathbf{y})$
- expected risk functional $R(\mathbf{Z},\mathbf{w})$

Goal: find the function $f(\mathbf{x}, \mathbf{w}_o)$ *minimizing* $R(\mathbf{Z},\mathbf{w})$ when the joint distribution $P(\mathbf{x},y)$ is *unknown.*

Empirical Risk Minimization

- ERM principle in model-based learning
  - Model parameterization: $f(\mathbf{x}, \mathbf{w})$
  - Loss function: $L(f(\mathbf{x}, \mathbf{w}),\mathbf{y})$
  - Estimate risk from data: $R_{emp}(\mathbf{w}) = \frac{1}{n}\sum_{i=1}^{n} L(f(\mathbf{x}_i, \mathbf{w}), y_i)$
  - Choose $\mathbf{w}^*$ that minimizes R_{emp}

- Statistical Learning Theory developed from the theoretical analysis of ERM principle under finite sample settings

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- **Statistical Learning Theory**
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Statistical Learning Theory

- History and Overview
- Conditions for consistency and convergence of ERM
- VC-dimension
- Generalization bounds
- Structural Risk Minimization (SRM) for learning with finite samples

History and Overview

- SLT aka **VC-theory** (Vapnik-Chervonenkis)
- Theory for estimating dependencies from finite samples (**predictive learning setting**)
- Based on the ***risk minimization*** approach
- All main results originally developed in 1970's for classification (pattern recognition)

  but remained largely unknown
- Renewed interest since late 90's due to practical success of **Support Vector Machines (SVM)**

History and Overview(cont'd)

MAIN CONTRIBUTIONS

- **Distinction** between problem setting, inductive principle and learning algorithms
- **Direct approach** to estimation with finite data (KID principle)
- **Math analysis of ERM** (inductive setting)
- **Two factors responsible for generalization:**

  - empirical risk (fitting/ training error)

  - complexity(capacity) of approximating functions

History and Overview(cont'd)

VC-theory has 4 parts:

1. Conditions for consistency/ convergence of ERM
2. Generalization bounds
3. Inductive principles (for finite samples)
4. Constructive methods (learning algorithms) for implementing (3)

NOTE: (1)→(2)→(3)→(4)

Consistency/Convergence of ERM

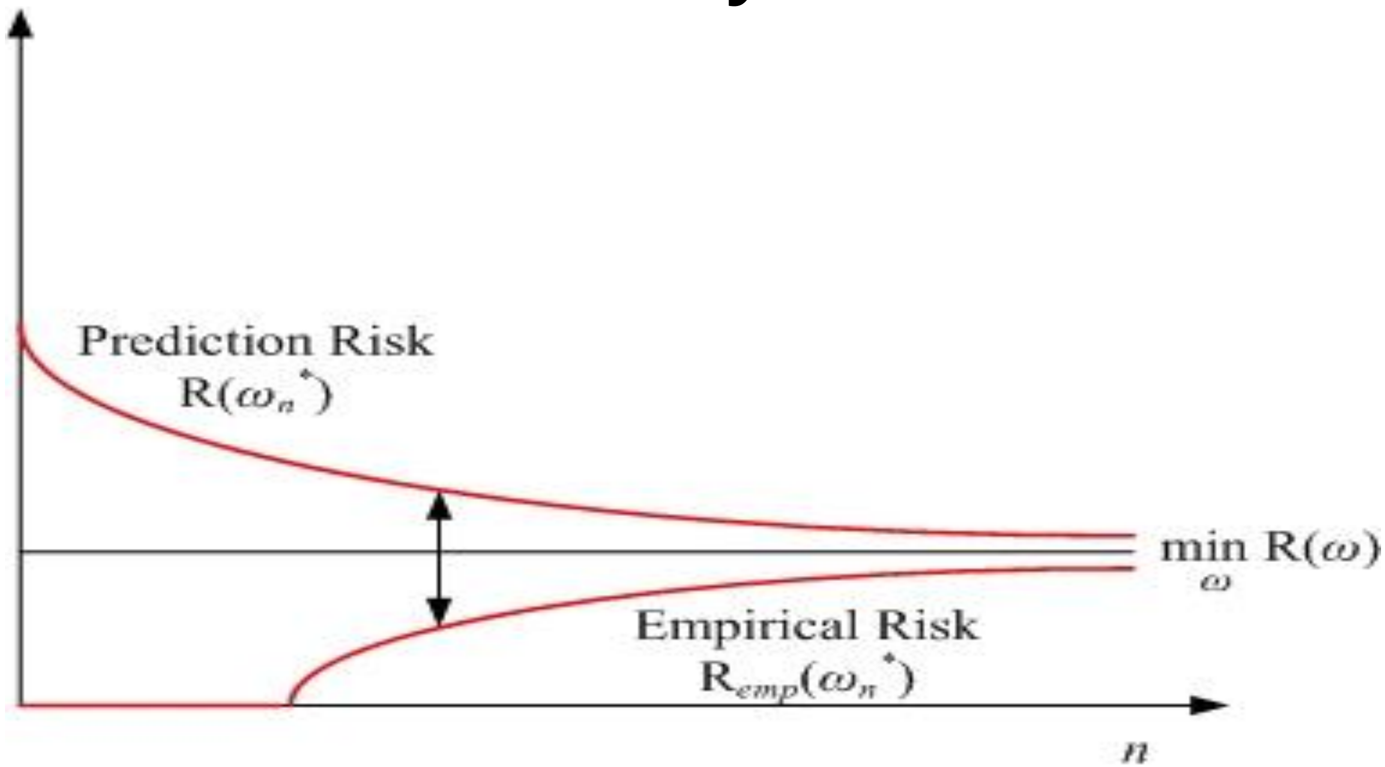
- Empirical Risk known but Expected Risk unknown
- **Asymptotic consistency requirement**:

  under what (general) conditions models providing *min Empirical Risk* will also provide *min Prediction Risk*, when the number of samples grows large?
- **Why asymptotic analysis** is important?

  - helps to develop useful concepts

  - necessary and sufficient conditions ensure that VC-theory is general and cannot be improved

Consistency of ERM



- Convergence of empirical risk $R_{emp}(\omega)$ *does not imply consistency* of ERM
- Models estimated via ERM (w*) are always *biased estimates* of the functions minimizing expected risk:

$$R_{emp}(\omega_n^*) < R(\omega_n^*)$$

Key Theorem of VC-theory

- For bounded loss functions, the ERM principle is consistent *if and only if* the empirical risk $R_{emp}(\omega)$ *converges uniformly* to the true risk $R(\omega)$ in the following sense

$$\lim_{n\to\infty} P[\sup_{\omega}\left|R(\omega)-R_{emp}(\omega)\right|>\varepsilon]=0, \forall\varepsilon>0$$

- consistency is determined by the *worst-case* approximating function, providing the largest discrepancy btwn the empirical risk and true risk

Note: this condition is not useful in practice. Need conditions for consistency in terms of general properties of a set of loss functions (approximating functions)

Conditions for Consistency of ERM

- **Goal**: to derive conditions for consistency & fast convergence in terms of the properties of loss functions
- Indicator 0/1 loss functions (binary classification)

$$Q(z,\omega) = \left| y - f(x,\omega) \right|$$

- Each indicator function partitions a given sample $Z_n = \{z_i\}, i = 1,2,\ldots n$ into two subsets (two classes). Each such partitioning is called dichotomy (二分法)
- The diversity $N(Z_n)$ of a set of functions $Q(z,\omega)$ is the number of different dichotomies that can be implemented on a random sample Z_n

  - the diversity is distribution-dependent

- The diversity $N(Z_n)$ (or capacity) needs to be bounded to ensure that a model can generalize well to unseen test data, not simply memorize the training data (e.g., one-nearest-neighbor).
- Following Vapnik (1995), we can further define the random entropy

$$H(\mathbf{Z}_n) = \ln N(\mathbf{Z}_n)$$

- Averaging the random entropy over all possible samples of size n generated from distrib. F(Z)

$$H(n) = E(\ln N(\mathbf{Z}_n))$$

- The VC entropy depends on the set indicator functions and on the (unknown) distribution of samples F(Z). => not good!

- The Growth Function is the maximum number of dichotomies that can be induced on a sample of size *n* (using the indicator fucntion)

$$G(n) = ln \max_{Z_n} N(Z_n)$$

since the max possible number *N* is 2^n

$$G(n) \leq n \ln 2$$

- The Growth Function is distribution-independent, and it depends only on the properties of a set of functions

$$Q(z, \omega)$$

- Another useful quantity is the Annealed VC entropy

$$H_{\text{ann}}(n) = \ln E(N(\mathbf{Z}_n))$$

By making use of Jensen's inequality,

$$\sum_i a_i \ln x_i \leq \ln\left(\sum_i a_i x_i\right)$$

it can be shown that

$$H(n) \leq H_{\text{ann}}(n)$$

- Hence, for any n the following inequality holds:

$$H(n) \leq H_{\text{ann}}(n) \leq G(n) \leq n \ln 2$$

- Vapnik and Chervonenkis (1968) obtained necessary and sufficient condition for consistency of the ERM principle in the form

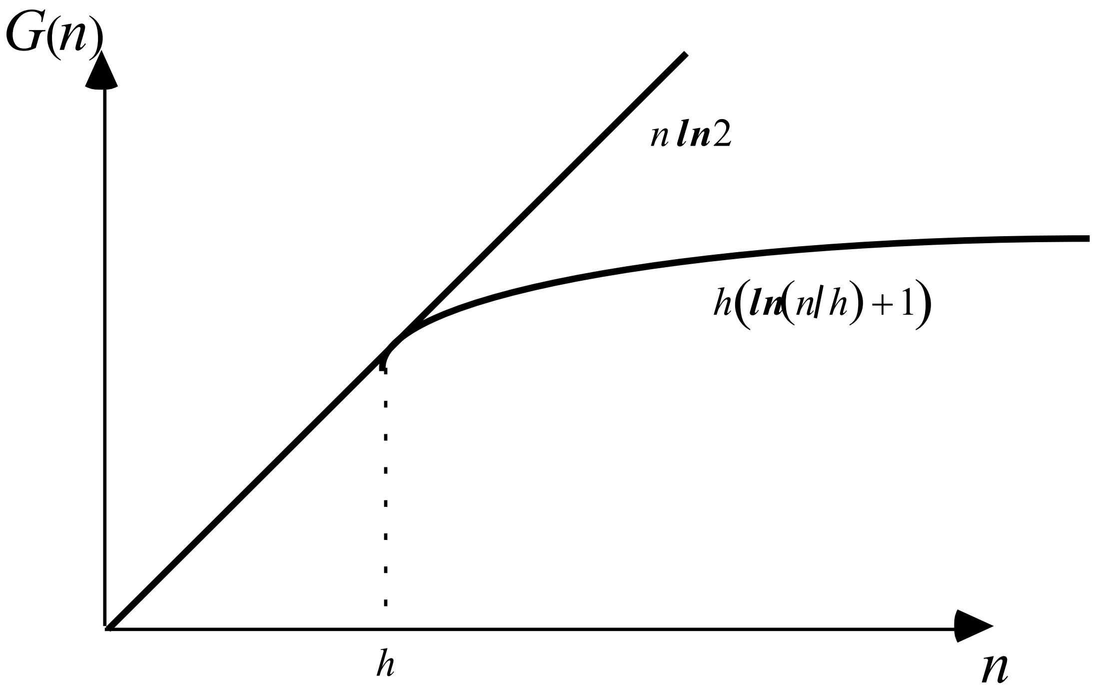
$$\lim_{n\to\infty} \frac{H(n)}{n} = 0$$

- SLT provides a distribution-independent condition (both necessary and sufficient) for consistency of ERM and fast convergence:

$$\lim_{n\to\infty} \frac{G(n)}{n} = 0$$

- This condition is distribution-independent.

Properties of the Growth Function (GF)



- **Theorem (**Vapnik & Chervonenkis, 1968): The Growth Function is either linear or bounded by a logarithmic function of the number of samples *n*.
- The point *n=h* where the GF starts to slow down is called **the VC-dimension** (of a set of indicator functions)

VC-dimension

- If the bound on the GF stays linear for any n:

  $G(n) = n \ln 2$ then the **VC-dimension is infinite**

  → *lim G(n)/n =* ln2 *and the ERM is* ***inconsistent****. That is, any sample of size n can be split in* 2^n *possible ways; hence no valid generalization is possible*

- Necessary and sufficient condition for consistency of ERM:

  Vapnik-Chervonenkis (VC) dimension is **finite**

  (this condition is distribution-independent)

- VC-dimension measures the ability (of a set of functions) to fit or ‘explain’ available finite data.

- VC-dimension of a set of indicator functions:

  - **Shattering**: if n samples can be separated by a set of indicator functions in all 2^n possible ways, then these samples can be shattered by this set of functions.

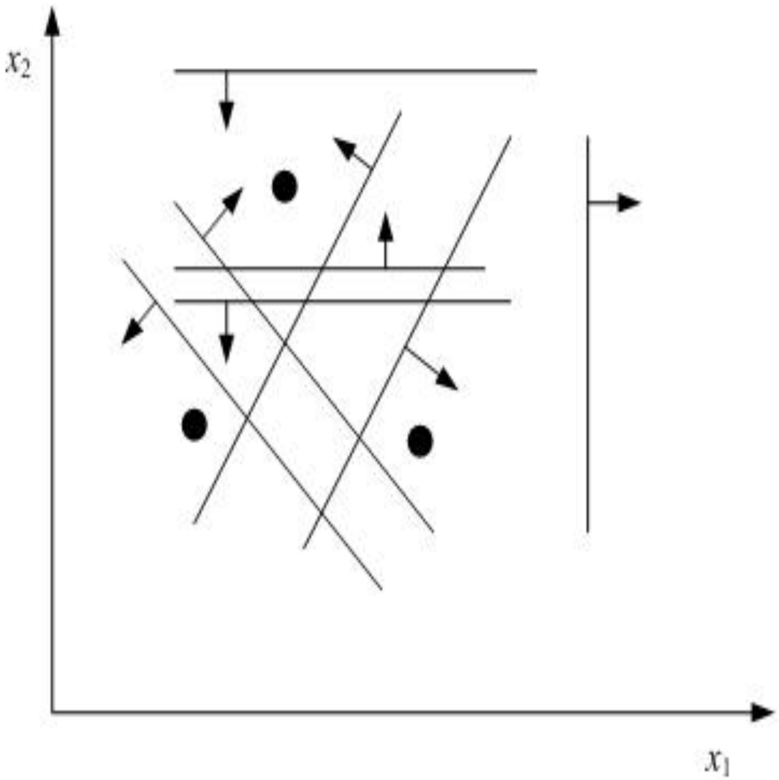
  - A set of functions has VC-dimension *h* if there exist *h* samples that *can be shattered* by this set of functions, but there *does not exist h+1 samples* that can be shattered.

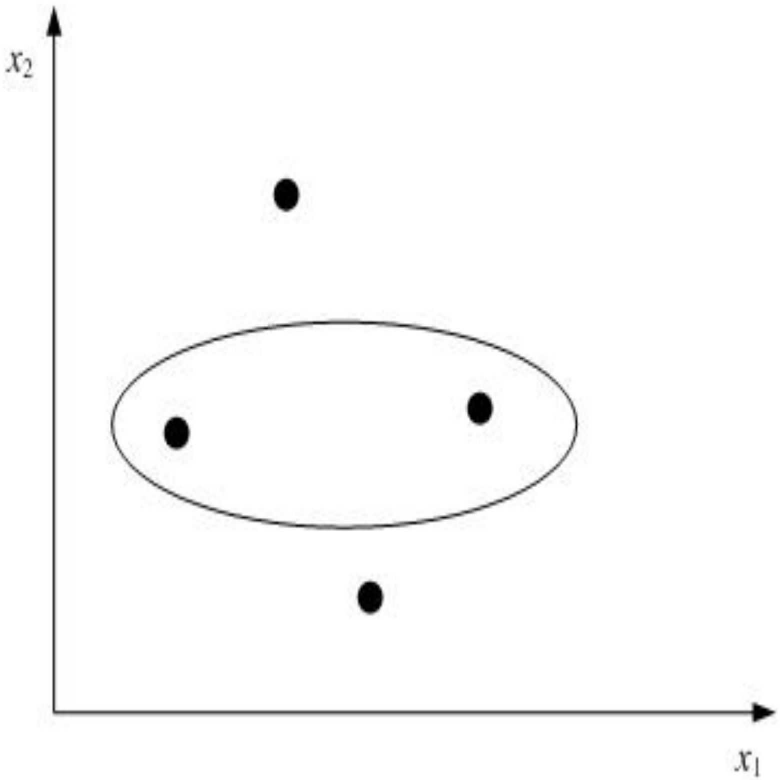
- Examples of analytic calculation of VC-dimension for simple sets of functions are shown next

- Linear Indicator Functions (d=2):

  there exist 3 points that can be shattered, but 4 cannot.

  → VC-dim. = 3.   In general, h=d+1



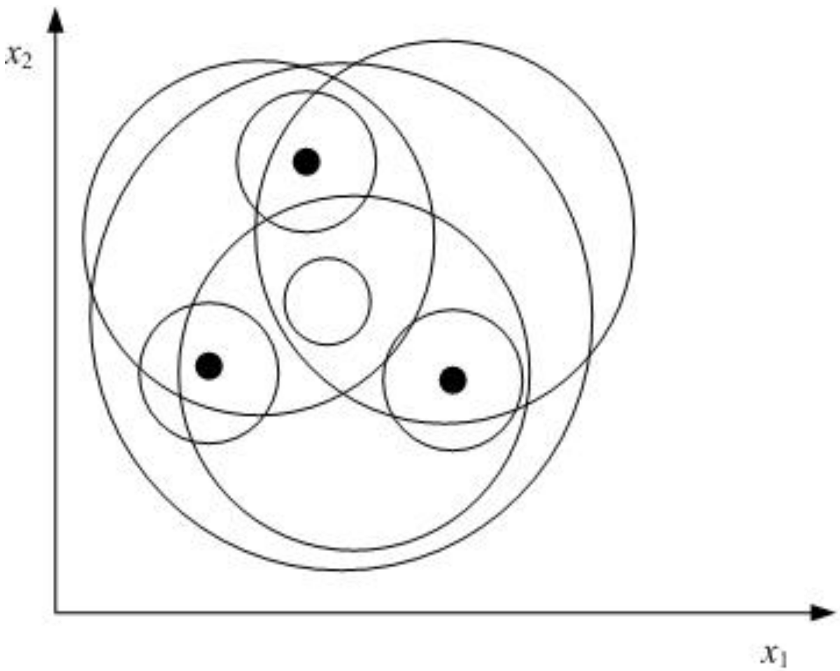


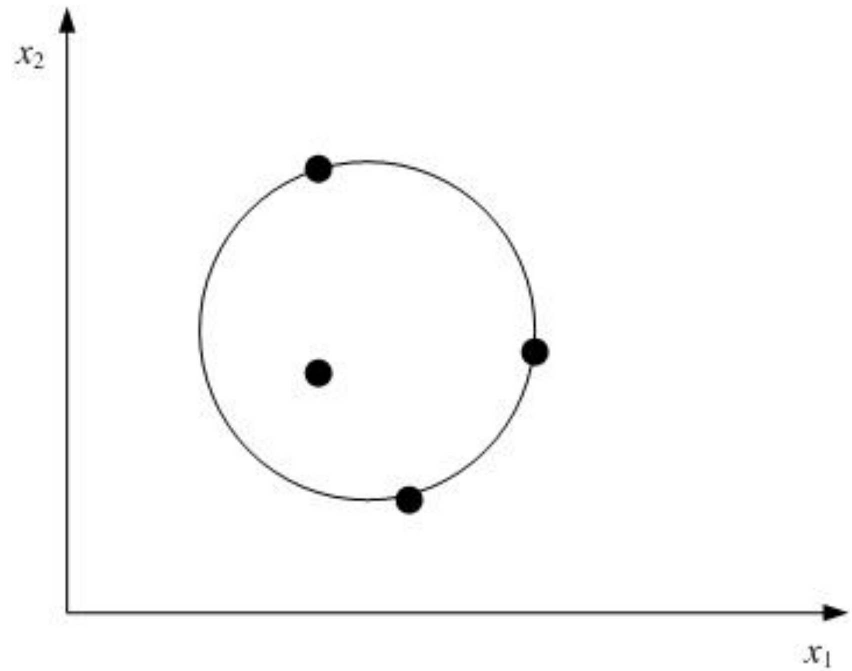
- Spherical (local) functions (d=2):

  there exist 3 points that can be shattered, but 4 cannot.

  → VC-dim. = 3.   In general, h=d+1

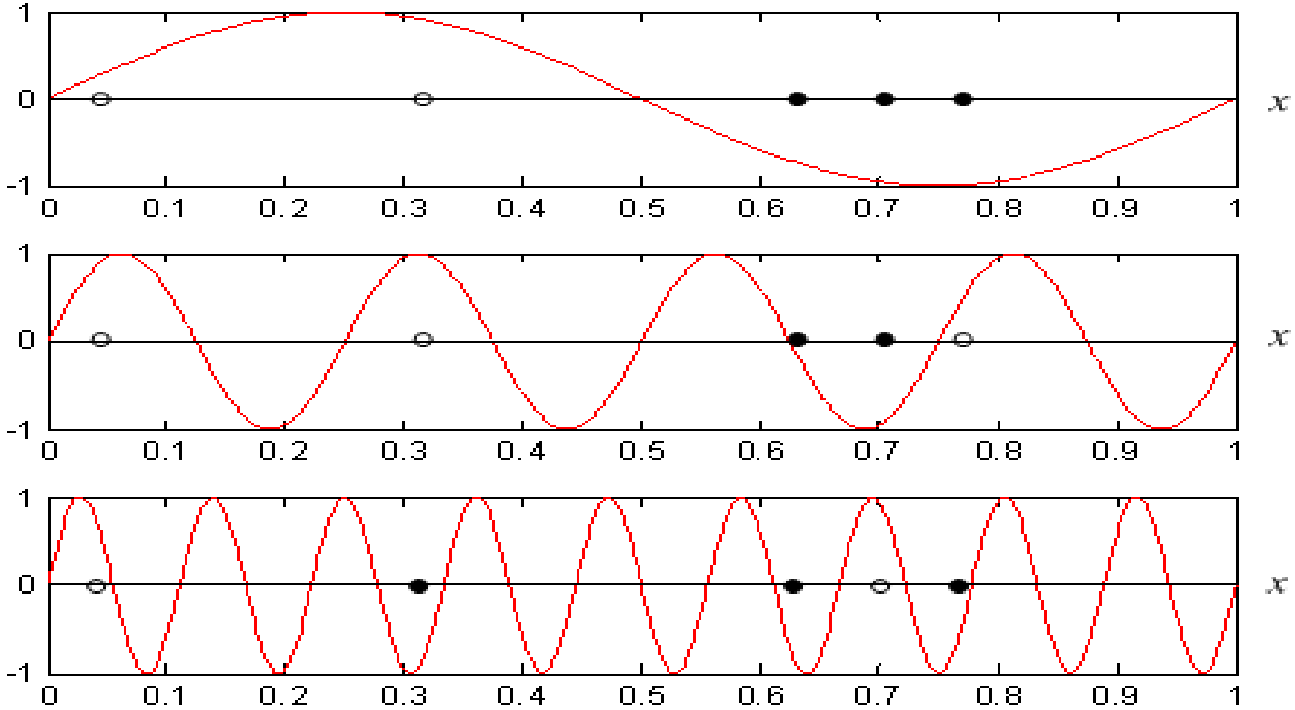
Note: in these examples, VC-dim = DoF (# of parameters)





- Example of infinite VC-dimension

  A set of indicator functions $y = I(\sin(\omega x))$ has infinite VC dimension



- Linear combination of fixed basis functions

$$f(\mathbf{x}, \mathbf{w}) = I\left(\sum_{i=1}^{m} w_i g_i(\mathbf{x}) + w_0 > 0\right)$$

is equivalent to linear functions in m-dimensional space

→ VC-dimension = m + 1

(this assumes linear independence of basis functions)

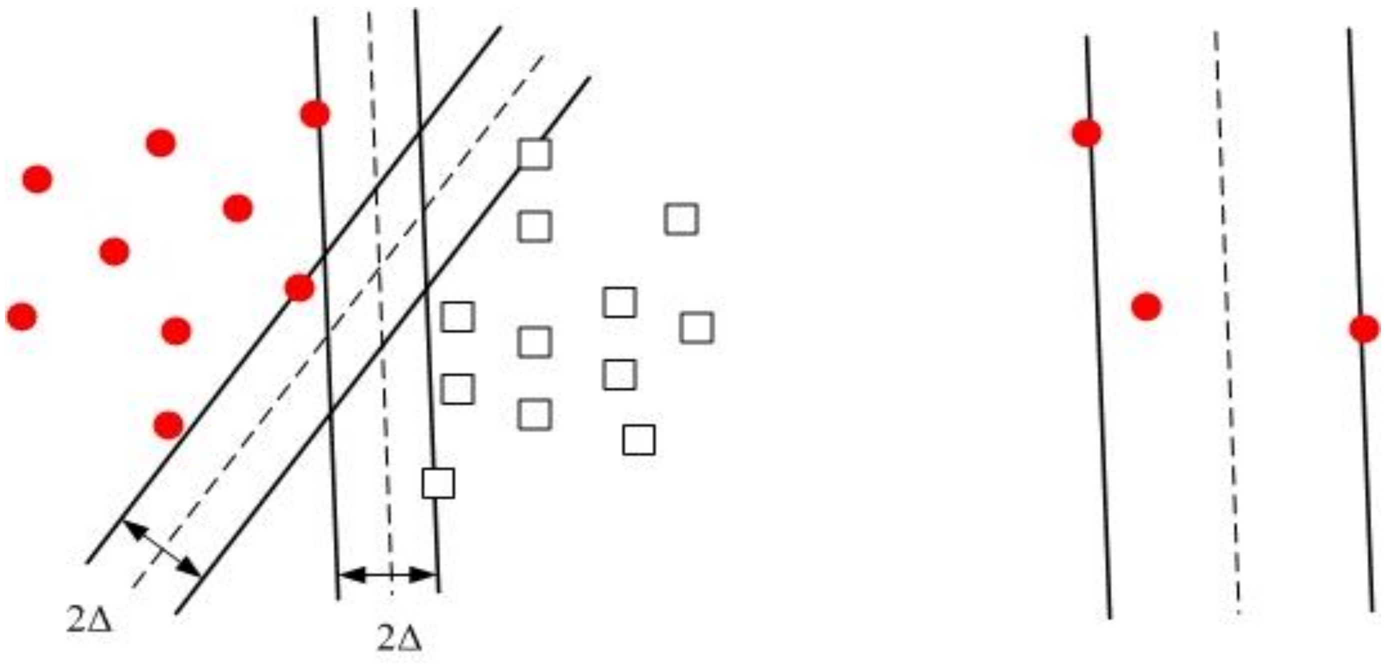
- In general, analytic estimation of VC-dimension is hard

- VC-dimension can be
  - equal to DoF
  - larger than DoF
  - smaller than DoF

- Delta-margin hyperplanes:

  consider linear slabs $D(\mathbf{x}) = (\mathbf{w} \cdot \mathbf{x}) + b$ separating samples from two classes, such that the distance btwn $D(\mathbf{x})$ and the closest data point is larger than some positive value Δ

- For large Δ, VC-dimension may be smaller than d+1:



VC-dimension and Falsifiability

- A set of functions has VC-dimension *h* if

(a) It can explain (shatter) a set of *h* samples
~ there exists *h* samples that cannot falsify it
and
(b) It can not shatter *h+1* samples
~ any *h+1* samples falsify this set

- *Finiteness of VC-dim* is necessary and sufficient condition for generalization
  (for *any* learning method based on ERM)

Philosophical interpretation: VC-falsifiability

- Occam's Razor: Select the model that explains available data *and* has the smallest number of free parameters (entities)

- VC theory: Select the model that explains available data *and* has low VC-dimension (i.e. can be easily falsified)

→ New principle of VC falsifiability

Generalization Bounds

- **Bounds for learning machines** (implementing ERM) evaluate the difference btwn (unknown) risk and known empirical risk, as a function of sample size *n* and the properties of the loss functions (approximating fcts).
- **Classification:** the following bound holds with probability of $1-\eta$ for all approximating functions

$$R(\omega) < R_{emp}(\omega) + \Phi\left(R_{emp}(\omega), n/h, -\ln\eta/n\right)$$

where Φ is called the confidence interval

- **Regression:** the following bound holds with probability of $1-\eta$ for all approximating functions

$$R(\omega) < R_{emp}(\omega) / \left(1 - c\sqrt{\varepsilon}\right)_+$$

where $$\varepsilon = \varepsilon\left(\frac{n}{h}, \frac{-\boldsymbol{ln}\,\eta}{n}\right) = a_1 \frac{h\left(\boldsymbol{ln}\frac{a_2 n}{h} + 1\right) - \boldsymbol{ln}(\eta/4)}{n}$$

Generalization Bounds (Practical form)

- **For classification (confidence level 1- η),**

$$R(\omega) \leq R_{\text{emp}}(\omega) + \frac{\varepsilon}{2}\left(1 + \sqrt{1 + \frac{4R_{\text{emp}}(\omega)}{\varepsilon}}\right)$$

  where $\varepsilon = \varepsilon\left(\frac{n}{h}, \frac{-\ln \eta}{n}\right) = a_1 \frac{h\left(\ln \frac{a_2 n}{h} + 1\right) - \ln(\eta/4)}{n}$

  practical choice: $a_1=a_2=1$

- **For regression (confidence level 1- η),**

$$R(\omega) \leq R_{\text{emp}}(\omega)\left(1 - \sqrt{p - p\ln p + \frac{\ln n}{2n}}\right)_+^{-1}$$

  where $p= h/n$

  practical choice:. $\frac{h}{n} \leq 0.8 \quad \text{for} \quad \eta \geq \min(4/\sqrt{n}, 1)$

- **large n => tight bound; small η=> loose bound.**

COMMENTS ON VC-BOUNDS

- **Useful** for conceptual understanding of general properties & limitations of all learning methods
- **Not appropriate** for practical use
- Properties of VC-bounds:

  - the confidence interval *monotonically* decreases to zero (*with n*)

  - bounds *depend strongly* on *n/h*;

  - bounds *do not depend* on dimensionality

Practical VC Bound for regression

- **Practical regression bound** can be obtained by setting the confidence level $\eta = min\left(4/\sqrt{n}, 1\right)$ and theoretical constants c=1, a1=a2=1 :

$$R(h) \le R_{emp}(h)\left(1 - \sqrt{\frac{h}{n} - \frac{h}{n}\ln\frac{h}{n} + \frac{\ln n}{2n}}\right)_{+}^{-1}$$

- Compare to analytic bounds (SC, FPE) in Lecture Set 2
- Analysis (of denominator) shows that

  ***h* < *0.8 n* for any estimator**

  In practice:

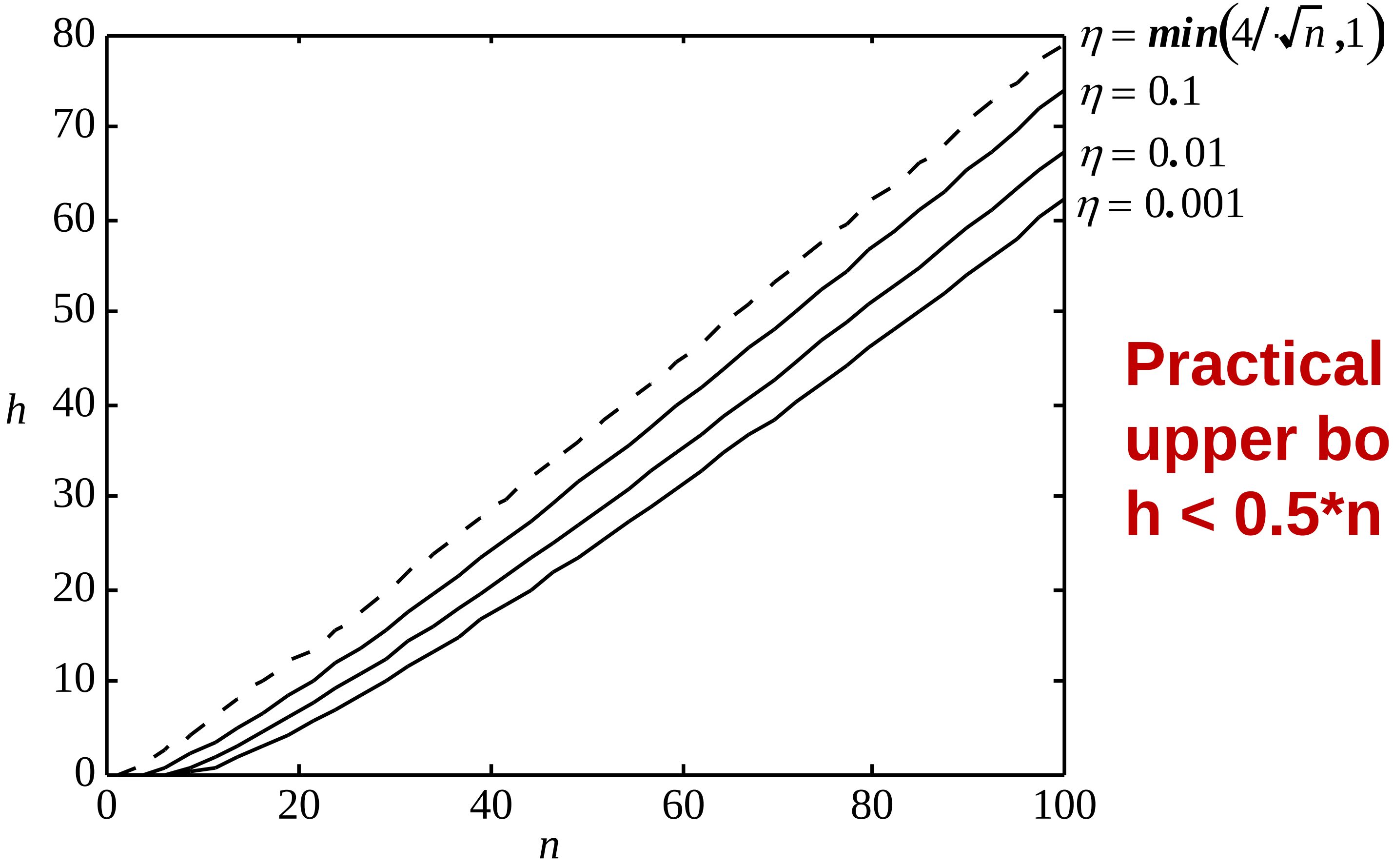
  ***h* < *0.5 n* for any estimator**

NOTE: generalization bounds *do not depend on dimension!*

Visual Illustration

- **Max possible *h* for given sample size *n***

for different confidence level values:



Practical upper bound h < 0.5*n

Structural Risk Minimization

- **Analysis of generalization bounds**

  $$R(\omega) < R_{emp}(\omega) + \Phi\left(R_{emp}(\omega), n/h, -\ln\eta/n\right)$$

  suggests that when *n/h* is large, the term Φ is small

  → $R(\omega) \sim R_{emp}(\omega)$

  This leads to parametric modeling approach (ERM)
- When *n/h* is not large (say, less than 20), both terms in the right-hand side of VC- bound need to be minimized

  → make the VC-dimension a controlling variable
- SRM = formal mechanism for controlling model complexity

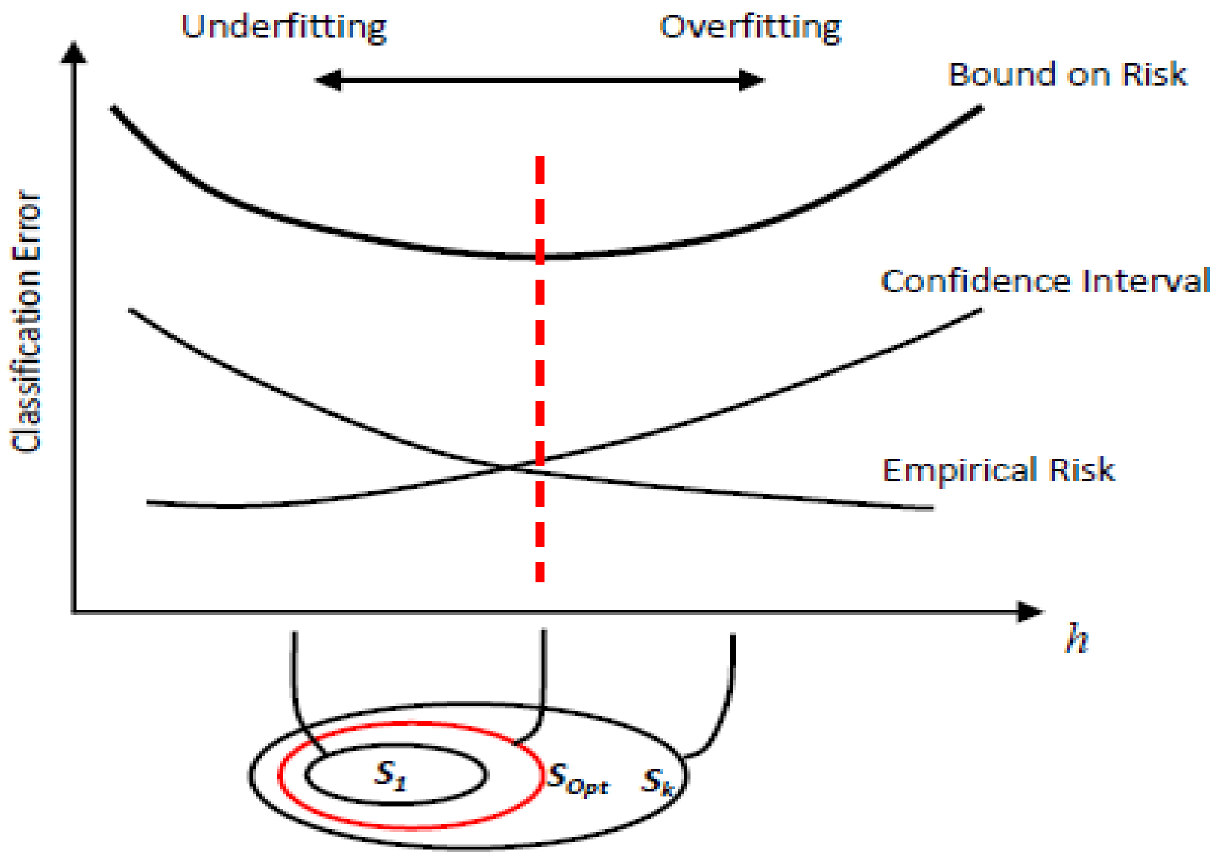
  Set of loss functions has nested structure $S_k = \{Q(\mathbf{z}, \omega), \omega \in \Omega_k\}$

  $S_1 \subset S_2 \subset \ldots \subset S_k \subset \ldots$ such that $h_1 \le h_2 \ldots \le h_k \ldots$

  → structure ~ complexity ordering

Structural Risk Minimization

- An upper bound on the true risk and the empirical risk, as a function of VC-dimension *h* (for fixed sample size *n*)



Structural Risk Minimization

- Contrast SRM vs ERM approach to data modeling

Given training examples $(\mathbf{x},y)$ sampled from unknown $P(\mathbf{x},y)$

Empirical Risk Minimization Modeling

1. Make assumptions about parameterization of admissible decision functions $f(\mathbf{x},\omega)$.
2. For each admissible model, estimate empirical risk (classification error) for the training data.
3. Select the classifier (decision function) providing smallest empirical risk.

Structural Risk Minimization Modeling

1. Introduce nested structure on a set of functions $f(\mathbf{x},\omega)$.
2. Minimize empirical risk for each element of a structure S_k.
3. Estimate guaranteed risk for each element S_k using VC- bounds.
4. Choose the best element S_0 providing smallest risk estimate, and select the function minimizing empirical risk on S_0 as the best model.

SRM Approach

- Use **VC-dimension** as a controlling parameter for minimizing VC bound:

$$R(\omega) < R_{emp}(\omega) + \Phi\left(n/h\right)$$

- **Two general strategies for implementing SRM**:

1. Keep $\Phi\left(n/h\right)$ fixed and minimize $R_{emp}(\omega)$
   (most statistical and neural network methods)

2. Keep $R_{emp}(\omega)$ fixed and minimize $\Phi\left(n/h\right)$
   (Support Vector Machines)

Common SRM structures

- **Dictionary structure**

A set of algebraic polynomials $\boldsymbol{f}_m(x, \mathbf{w}) = \sum_{i=0}^{m} w_i x^i$

is a structure since $\boldsymbol{f}_1 \subset \boldsymbol{f}_2 \subset \ldots \subset \boldsymbol{f}_k \subset \ldots$

More generally $\boldsymbol{f}_m(\mathbf{x}, \mathbf{w}, \mathbf{V}) = \sum_{i=0}^{m} w_i \, \boldsymbol{g}(\mathbf{x}, \mathbf{v}_i)$

where $\boldsymbol{g}(\mathbf{x}, \mathbf{v}_i)$ is a set of basis functions (dictionary).

The number of terms (basis functions) *m* specifies an element of a structure.

For fixed basis fcts, VC-dim = number of parameters w_i

Common SRM structures (cont'd)

- **Feature selection** (aka subset selection)

  Consider sparse polynomials $f_m(x, \mathbf{w}) = \sum_{i=0}^{m} w_i x^{k_i}$

  where k_i is a (positive) integer

  Each monomial is a feature → the goal is to select a set of *m* features providing min. empirical risk (MSE)

  This is a structure since $f_1 \subset f_2 \subset .... \subset f_m \subset ....$

  More generally, representation $\boldsymbol{f}_m(\mathbf{x}, \mathbf{w}, \mathbf{V}) = \sum_{i=0}^{m} w_i \, \mathbf{g}(\mathbf{x}, \mathbf{v}_i)$

  where *m* basis functions are selected from a large (given) set of M functions

Note: nonlinear optimization, VC-dimension is unknown

Common SRM structures (cont'd)

- **Penalization**

Consider algebraic polynomial of fixed degree

$$f(x,\mathbf{w}) = \sum_{i=0}^{10} w_i x^i \quad \text{where} \quad \|\mathbf{w}\|^2 \le c_k \qquad c_1 < c_2 < c_3 \ldots$$

For each (positive) value c this set of functions specifies an element of a structure $S_k = \{\, f(\mathbf{x},\mathbf{w}),\ \|\mathbf{w}\|^2 \le c_k \,\}$

Minimization of empirical risk (MSE) on each element S_k of a structure is a constrained minimization problem

This optimization problem can be equivalently stated as minimization of the penalized empirical risk functional:

$R_{pen}(\omega,\lambda_k) = R_{emp}(\omega) + \lambda_k \|\mathbf{w}\|^2$ where the choice of $\lambda_k \sim c_k$

Note: VC-dimension is unknown

Common SRM structures (cont'd)

- **Initialization structure**

  The structure is defined for nonlinear optimization algorithm A fitting training data using a set of functions $f(\mathbf{x},\mathbf{w})$ with initial conditions $\mathbf{w}_0$

  $S_k = [A: f(\mathbf{x},\mathbf{w}),\ \|\mathbf{w}_0\| < C_k]$ where $C_1 < C_2 < \ldots$

- **Early stopping rules**

  The structure is defined for nonlinear optimization algorithm A fitting training data. The structure is index by the *number of iterative steps* of algorithm A, starting with initial (small) values of parameters $\mathbf{w}_0$

Common SRM structures (cont'd)

- **Margin-based structure**

  Recall large-margin separating hyperplanes for classification.

  Larger-margin hyperplanes form a subset of all *smaller-margin* hyperplanes:

$$S_{\Delta 1} \subset S_{\Delta 2} \subset \ldots \subset S_{\Delta k} \subset \ldots$$

for $\Delta 1 > \Delta 2 > \ldots.$

→ VC-dimension controlled by margin size Δ

Example of SRM for Regression

- Polynomial regression using different structures

  Regression problem: $y = 0.8\sin(2\pi\sqrt{x}) + 0.2x^2 - 0.5\sqrt{x} + \xi$

  x-values uniform on [0,1], Gaussian noise $\sigma = 0.05$

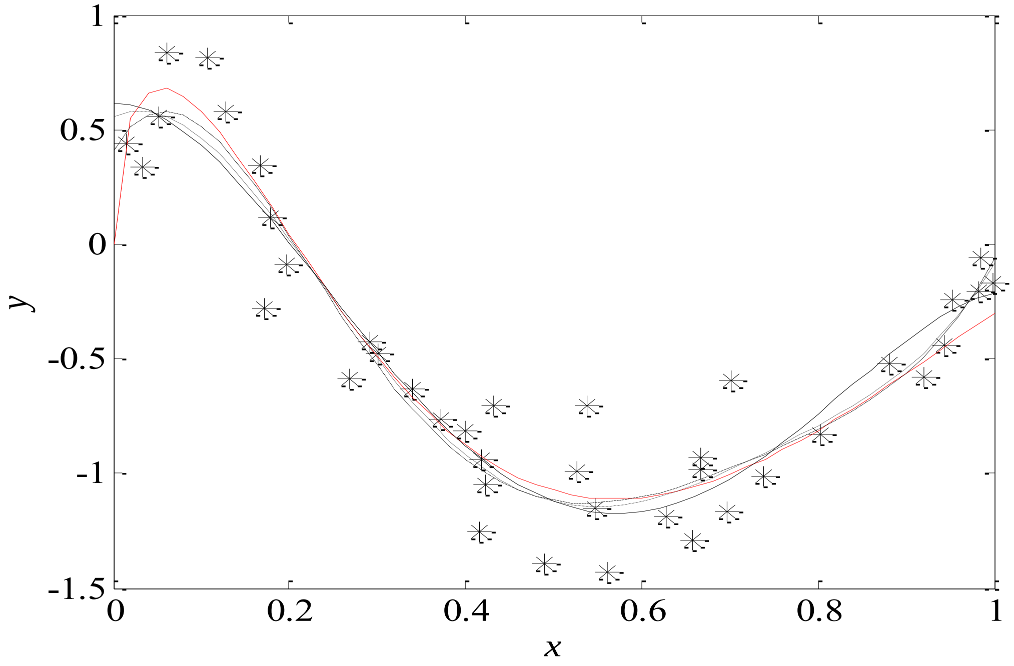
  training set ~ 40 samples; validation ~ 40 samples
- Different structures

  - dictionary (degrees 1 to 10)

  - penalization (degree 10 with ridge penalty)

  - sparse polynomials (of degree 1 to 6)

- Dictionary $\hat{y} = 0.4078 + 6.4198x - 68.2162x^2 + 163.7679x^3 - 158.3952x^4 + 55.9565x^5$
- Penalization *lambda = 1.013e-005*
- Feature selection $\hat{y} = 0.6186 - 22.7337x^2 + 41.1772x^3 - 19.2736x^4$



target function ~ red line; dictionary ~ black dashed;

penalization ~ black dotted; feature selection ~ black solid

Aside: model interpretation

- **Outside the scope of VC-theory**
- **In the last example:**

  different structures on the *same set of functions*

  lead to different interpretations

- Often interpretation assumes function identification setting
- In practice, interpretation always requires application domain knowledge

Practical Implementation of SRM

- **Need to**

  - estimate VC-dim for an element of a structure Sk

  - minimize empirical risk for each element Sk

- **Both possible** for linear approximating functions

- **Both difficult** for nonlinear parameterization

  → many heuristic learning algorithms

SRM structures: summary

- **SRM structure** ~ complexity ordering on a set of admissible models (approximating functions)
- **Many different structures** on the same set of approximating functions

  Which one is the 'best'?

  - depends on the properties of application data

  - can be decided via empirical comparisons
- **SRM = mechanism for complexity control**

  - selecting optimal complexity for a given data set

  - new measure of complexity: VC-dimension

  - model selection using analytic VC-bounds

OUTLINE

- Objectives
- Inductive learning problem setting
- Statistical Learning Theory
- **Applications**
  - model selection (for regression)
  - market timing of international funds
  - signal denoising
- Measuring the VC-dimension
- Summary and discussion

Application: VC-based model selection

see http://www.mitpressjournals.org/toc/neco/15/7

- Standard regression setting $y = g(\mathbf{x}) + noise$
- Statistical criteria

- Akaike Information Criterion (**AIC**)

$$AIC(d) = R_{emp}(d) + \frac{2d}{n}\hat{\sigma}^2$$

- Bayesian Information Criterion (**BIC**)

$$BIC(d) = R_{emp}(d) + (\ln n)\frac{d}{n}\hat{\sigma}^2$$

where *d* ~ (effective) DoF, *n* ~ sample size

- Require noise estimation $\hat{\sigma}^2 = \frac{n}{n-d} \cdot \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$

- Many methods require noise estimation

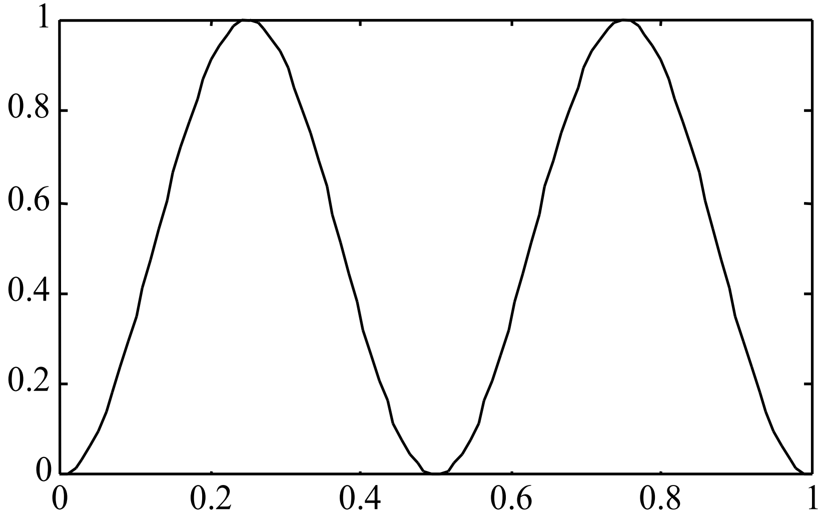
$$\hat{\sigma}^2 = \frac{n}{n-h} \cdot \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 = \frac{n}{n-h} R_{emp}$$

- One approach is to estimate noise for each (fixed) model complexity → multiplicative criteria
- Another approach is to estimate noise first and then use it in the additive AIC or BIC criteria
- This study uses additive AIC/BIC assuming known noise variance
- **VC-based model selection (aka *VM*)**

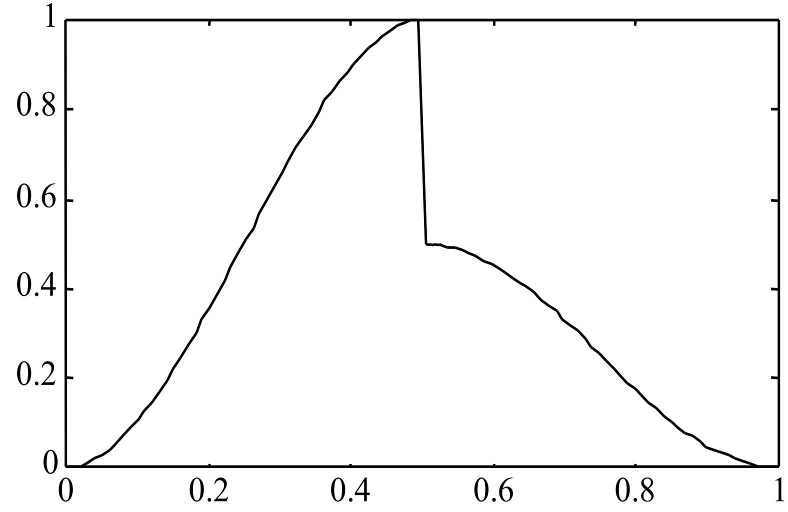
$$R(h) \le R_{emp}(h)\left(1 - \sqrt{\frac{h}{n} - \frac{h}{n}\ln\frac{h}{n} + \frac{\ln n}{2n}}\right)_+^{-1}$$

Comparison for univariate regression

(a) Sine squared function $sin^2(2\pi x)$

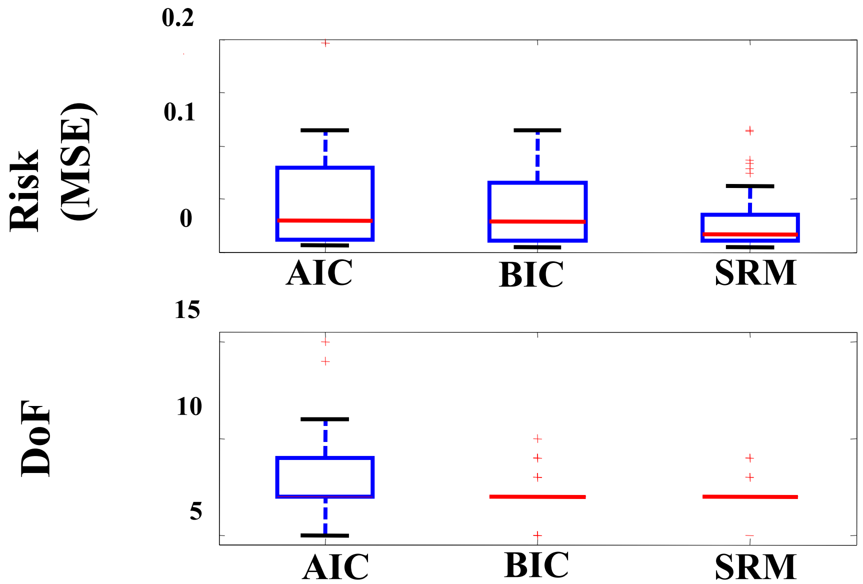


(b) Piecewise polynomial



- Target functions: continuous + discontinuous
- Approximating functions: algebraic polynomials
  Fourier basis

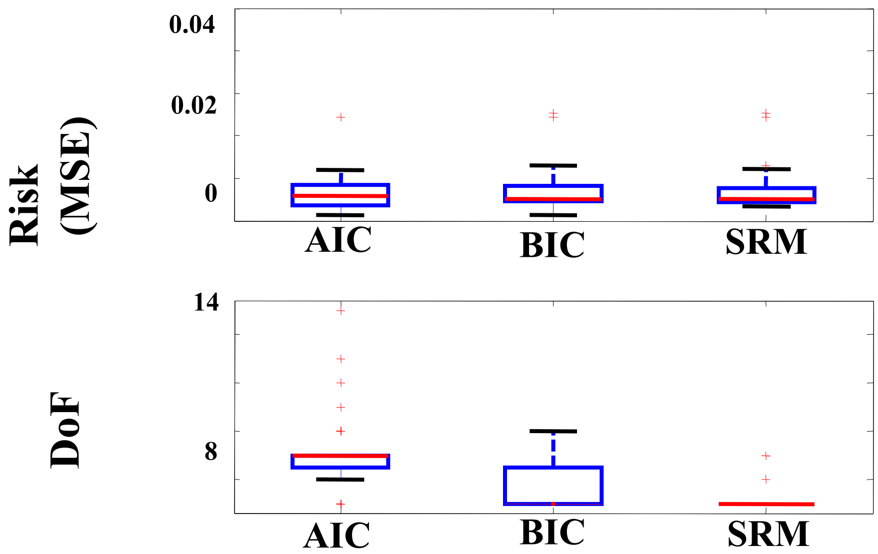
Sine-squared target fct, polynomial regression sample size *n*=30, noise $\sigma = 0.2$



Comparison of AIC, BIC & SRM (or VM):

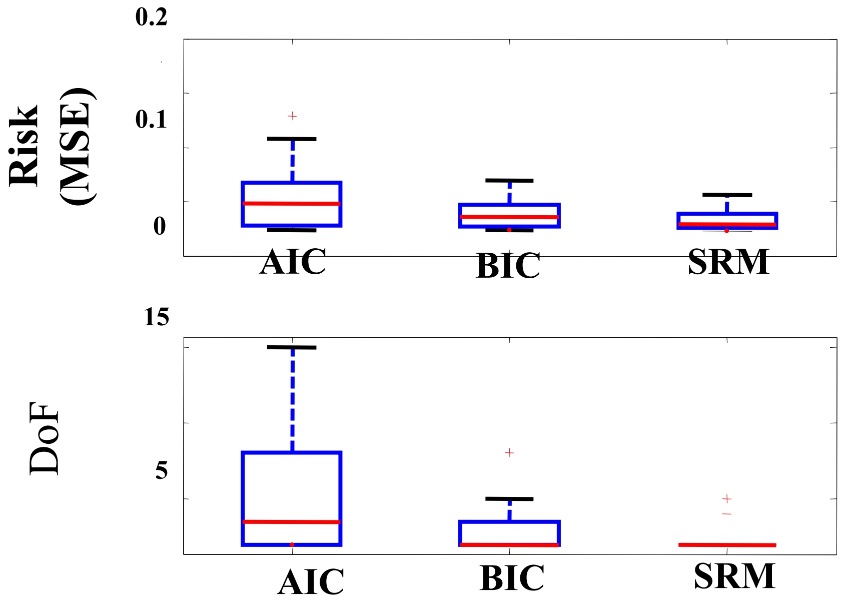
- prediction risk (MSE)
- selected DoF (~ h)

Sine-squared target fct, polynomial regression sample size n=100, noise $\sigma = 0.2$



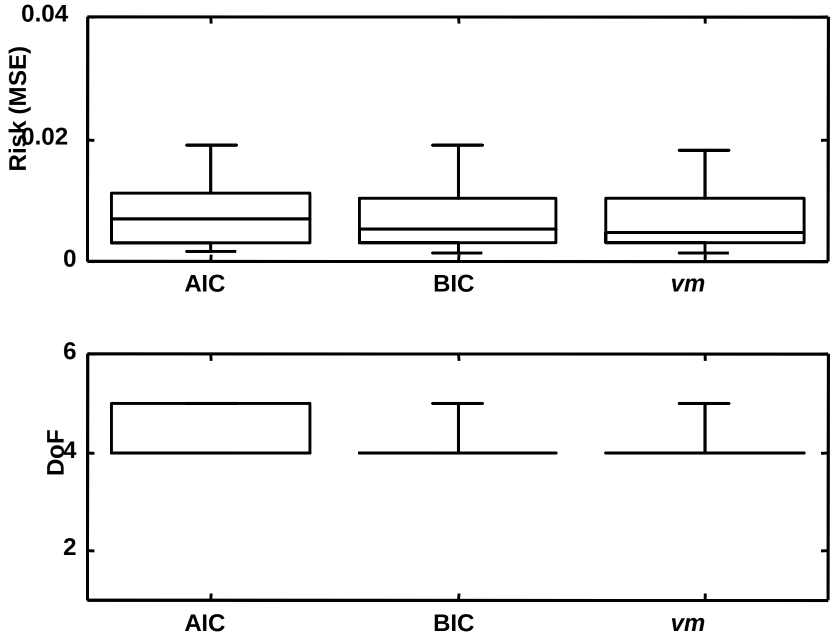
Better model selection approaches select models providing lowest guaranteed prediction risk (i.e. with lowest risk at the 95 percent mark) and also smallest variation of the risk (i.e., narrow box plots).

Piecewise polynomial, Fourier estimation sample size *n*=30, noise $\sigma = 0.2$



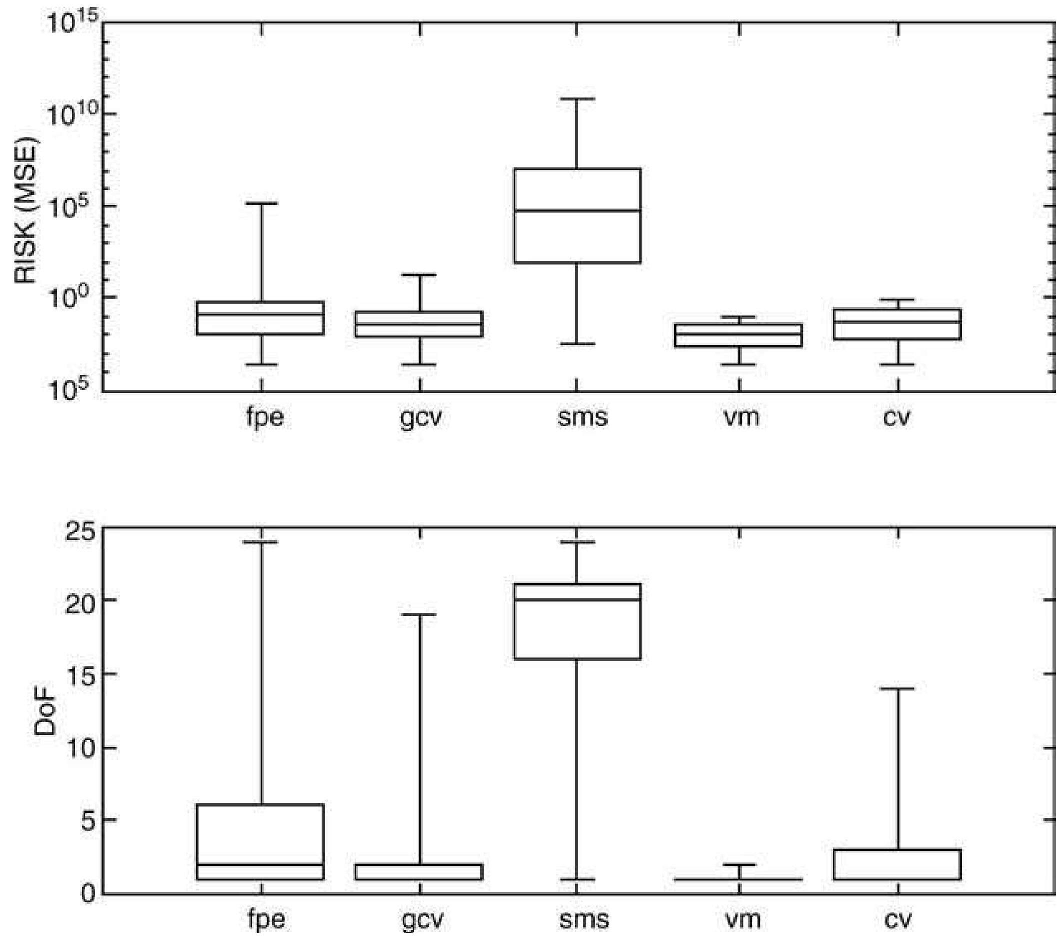
Comparison for linear subset selection

- Target function: $y = x_1 + 2x_2 + x_3 + 0 * x_4 + 0 * x_5 + \xi$
- x-values uniform in [0,1], *n*=30 samples
  gaussian noise $\sigma = 0.2$
- Approximating functions: linear subset selection



Unknown target function with pure Gaussian noise.

- Model selection results for sample size 30.
- Using algebraic polynomial estimators.
- The true model is the mean of training samples (DoF = 1).
- VC based model selection typically selects the ‘‘correct’’ model (DoF = 1).



Lots of confusion about model selection

- Cherkassky et al (1999): VC-analytic bound works very well for (univariate) regression problems

  Hastie et al (2001): SRM (using VC-bound) performs poorly overall

See http://www.mitpressjournals.org/toc/neco/15/7

- What is the cause for disagreement?

  - technical sloppiness + lack of common sense

- More confusing studies are generated each year

See http://www.springerlink.com/content/kq4g614j3xhdupuu/fulltext.pdf

Discussion question: read the paper Sugiama & Ogawa(2002) and try to understand the deficiencies in their experimental procedure and/or assumptions used in this paper.

Market Timing of International Funds: A Decade after the Scandal

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University of Minnesota
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Presented at CIFEr, March 30, 2012

OUTLINE

- **Motivation + Background**
  - mutual fund basics
  - scandals in early 2000's
  - regulations on frequent trading

- Predictive (VC-theoretical) methodology
- Empirical Results: market timing of TWIEX
- Conclusions and policy implications

Timing of International Funds

- **International mutual funds**

  - priced at 4 pm EST

  - reflect price of foreign securities traded at European/ Asian markets

  - Foreign markets close earlier than US market

→ **Possibility of inefficient pricing**

Market timing exploits this inefficiency.

- **Logical solution:** implement efficient pricing [Zitzewitz 2003]
- **Solution adopted:** restrictions on trading

Data Analytic Approach

- **Timing of international mutual funds**

  Can it be consistently profitable under

  - past market conditions ? (2004 ~ 2005)

  - current market conditions ? (2009 ~ 2012)

- **Predictive data modeling:**

  - estimate trading model (using past data)

  - apply this model for prediction (trading)

- **Diversified international fund** (TWIEX)

  American Century Int'l Growth Fund

Binary Classification Setting

- TWIEX ~ American Century Int'l Growth
- ***Input indicators*** (for trading) ~ today
  - SP 500 index (daily % change) ~ x_1
  - Euro-to-dollar exchange rate (% change) ~ x_2
- ***Output*** : TWIEX NAV (% change) ~next day

- ***Model parameterization*** (fixed):
  - linear $g(\mathbf{x}, \mathbf{w}) = w_1 x_1 + w_2 x_2 + w_0$
  - quadratic $g(\mathbf{x}, \mathbf{w}) = w_1 x_1 + w_2 x_2 + w_3 x_1^2 + w_4 x_2^2 + w_5 x_1 x_2 + w_0$
- ***Decision rule*** (estimated from training data):

$$D(\mathbf{x}) = Sign(g(\mathbf{x}, \mathbf{w}^*))$$

VC theoretical Methodology

- **When a trained model can predict well?**

(1) Future/test data is similar to training data

i.e., use 2004 period for training, and 2005 for testing

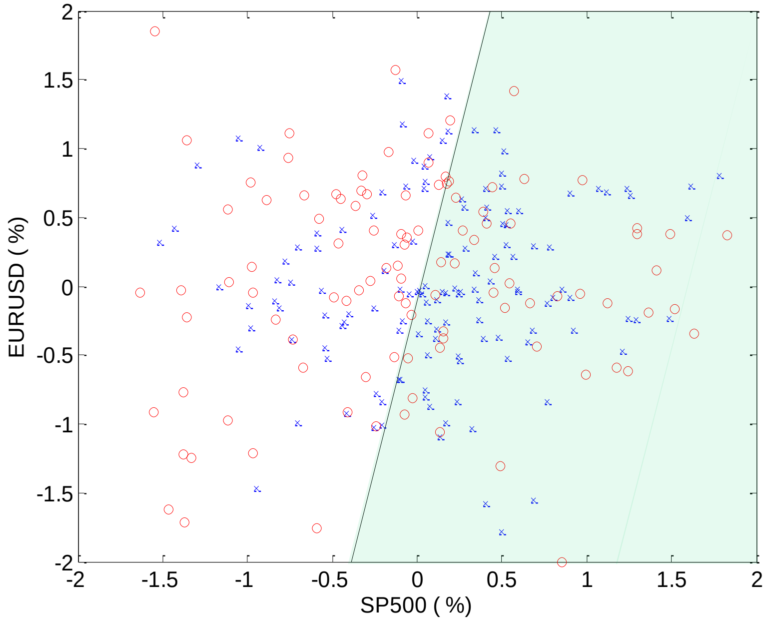
(2) Estimated model is 'simple' *and* provides good performance during training period

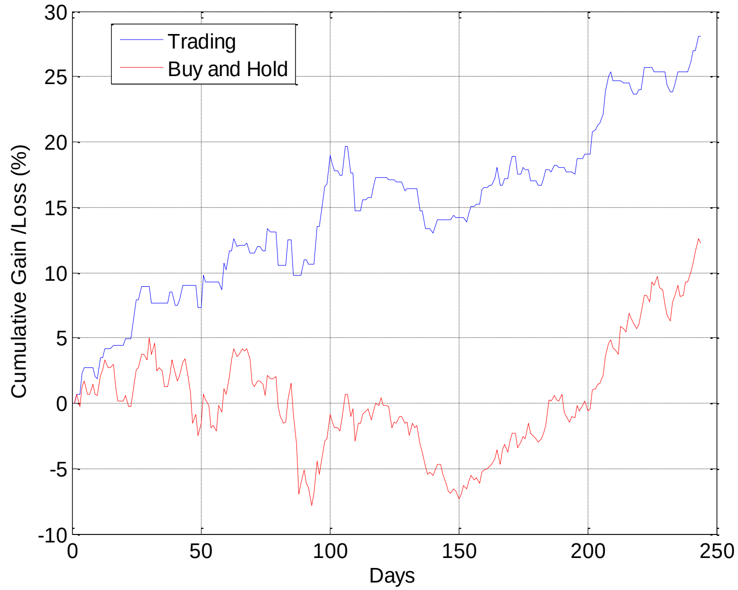
i.e., trading strategy is *consistently better* than *buy-and-hold* during training period

Empirical Results: 2004 -2005 data

Linear model

Training data 2004   Training period 2004



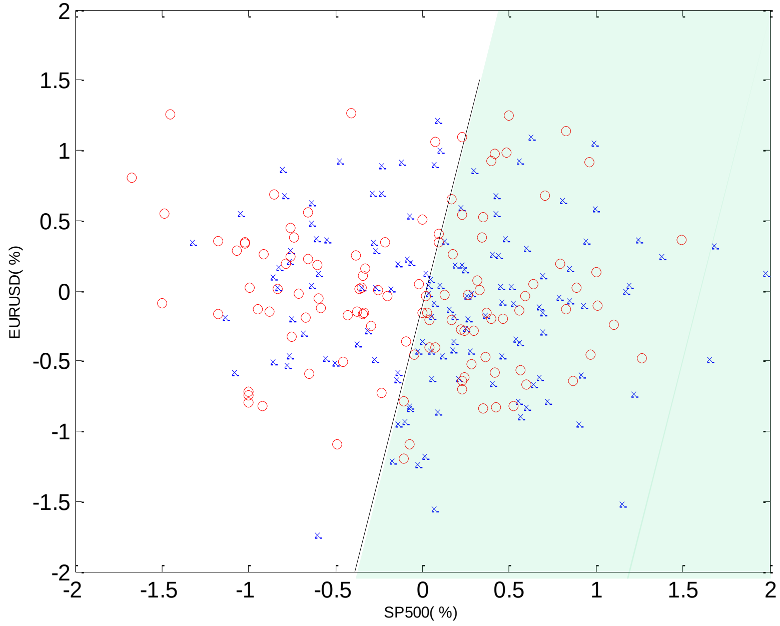


→ can expect good performance with test data

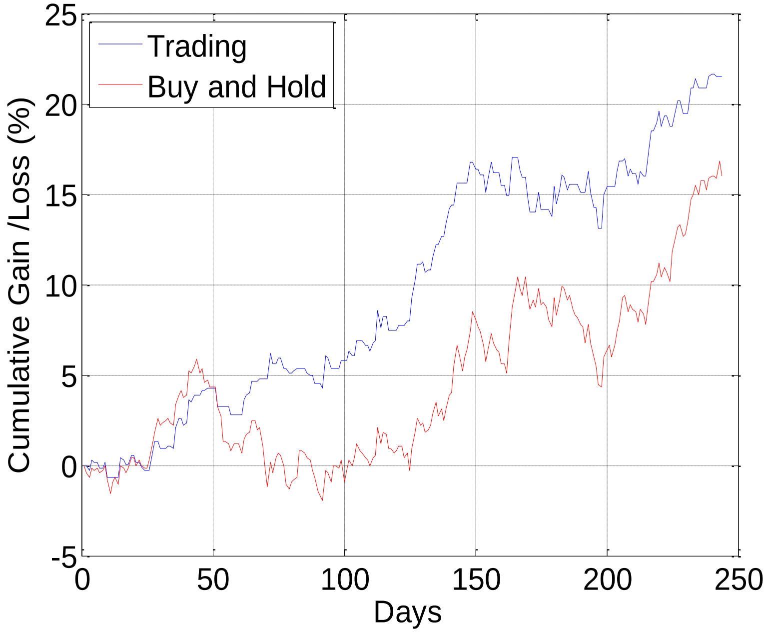
Empirical Results: 2004 -2005 data

Linear model

Test data 2005



Test period 2005

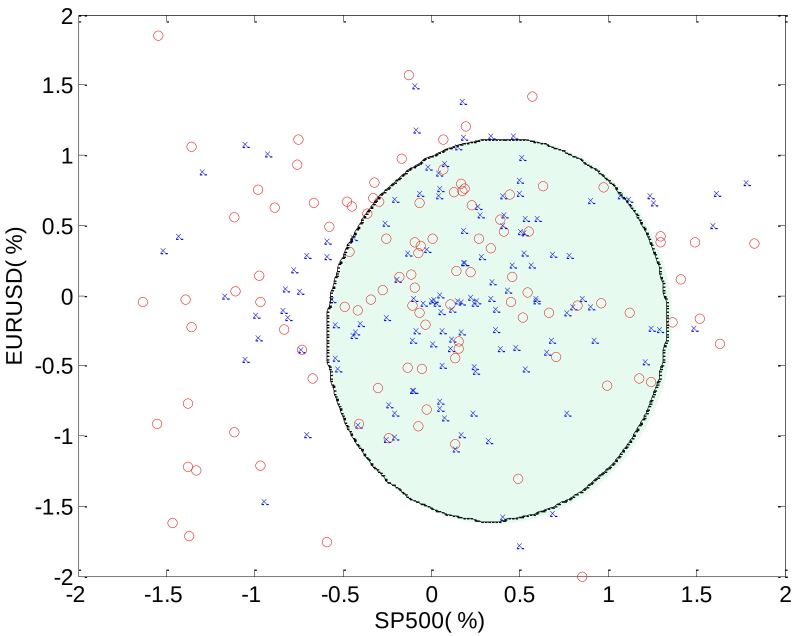


confirmed good prediction performance

Empirical Results: 2004 -2005 data

Quadratic model

Training data 2004 | Training period 2004

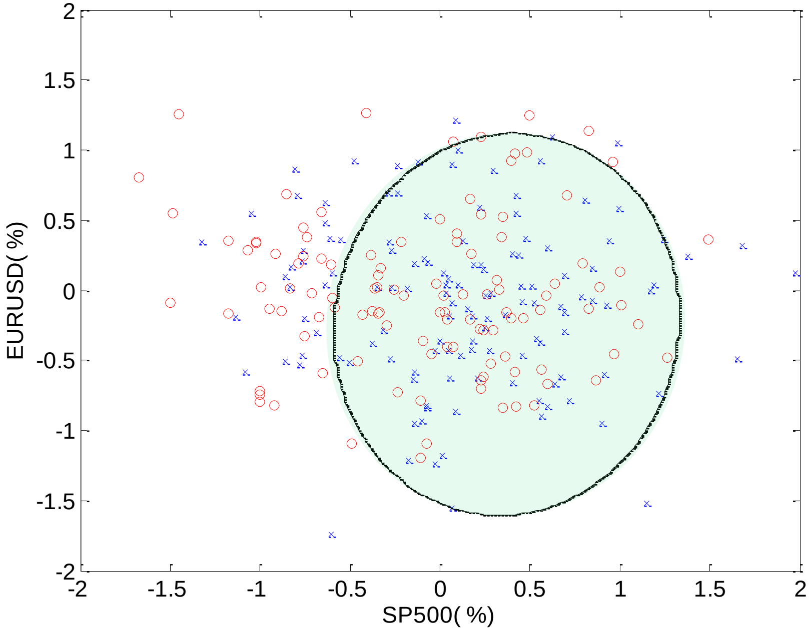


→ can expect good performance with test data

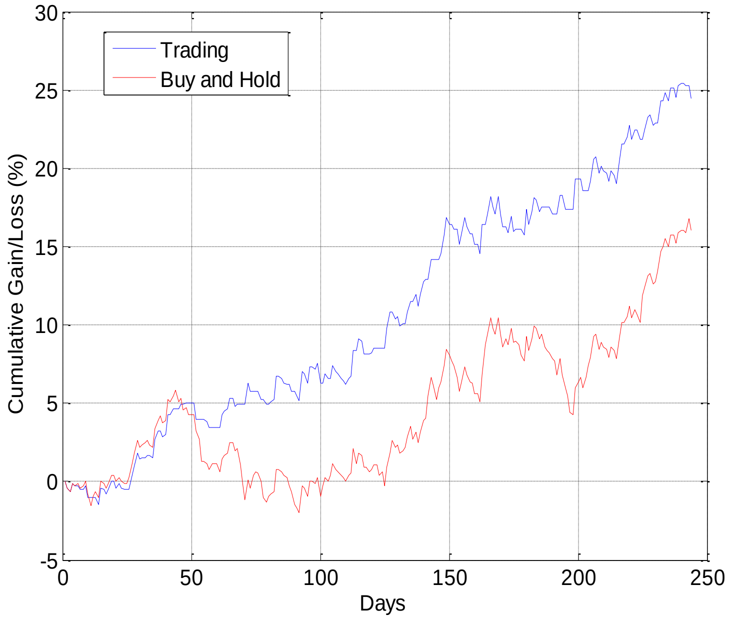
Empirical Results: 2004 -2005 data

Quadratic model

Test data 2005



Test period 2005

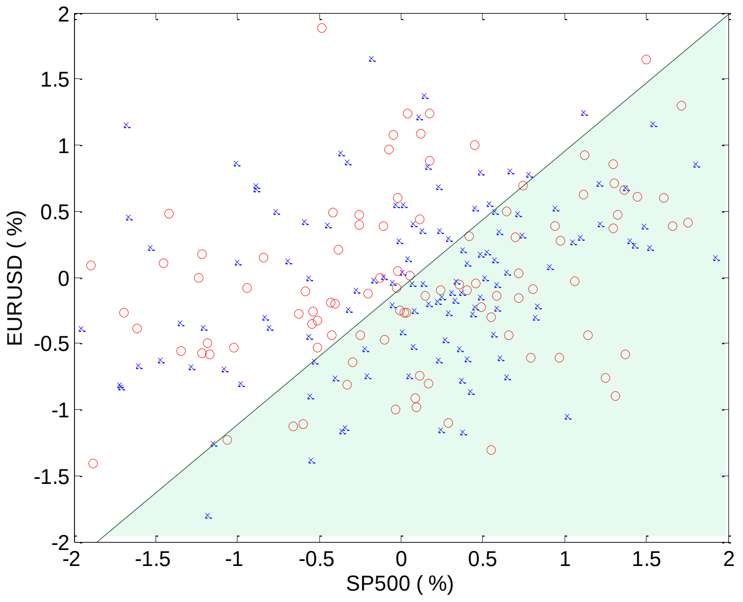


confirmed good test performance

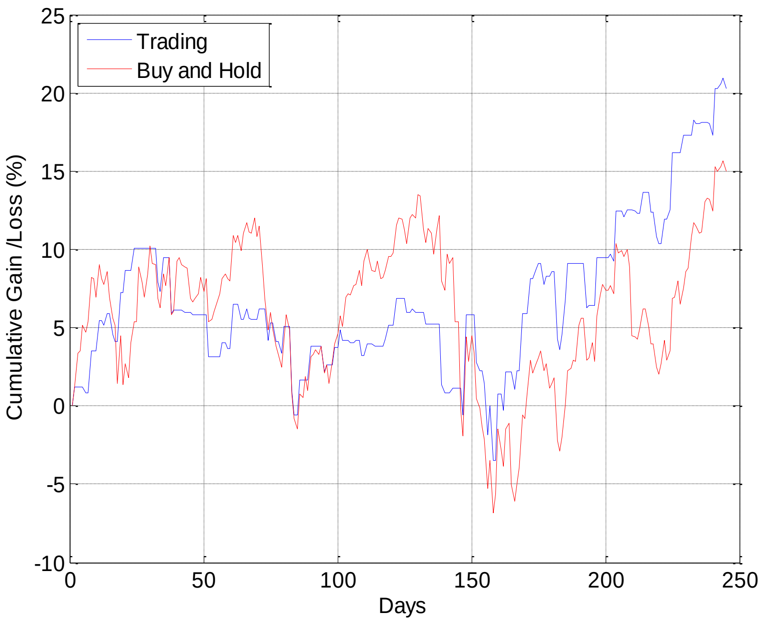
Empirical Results: 2010 -2011 data

Linear model

Training data 2010



Training period 2010



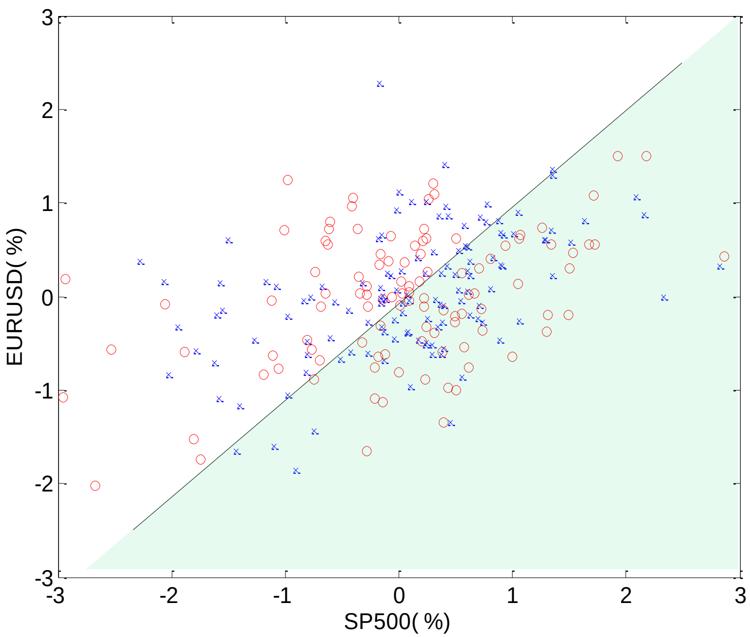
→ performance is *no better* than buy-and-hold

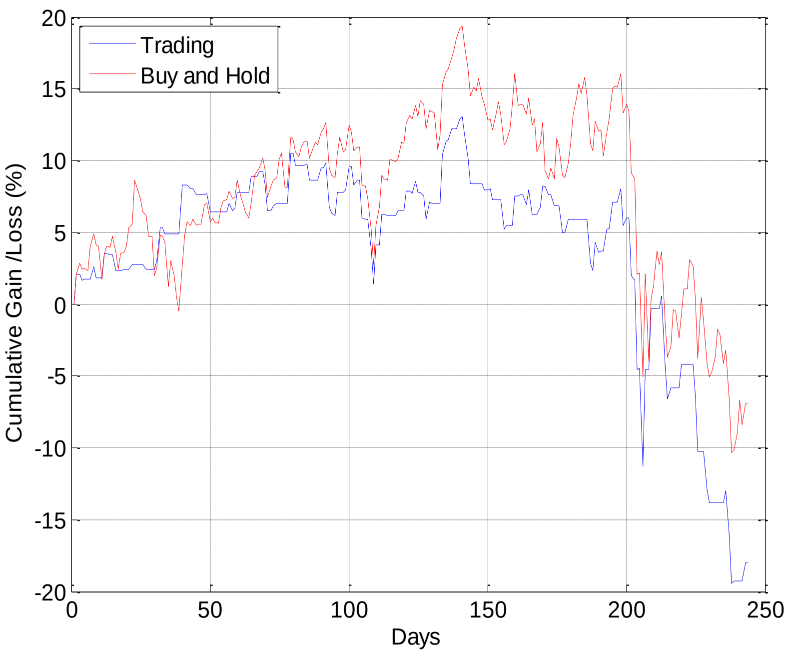
Empirical Results: 2010 -2011 data

Linear model

Test data 2011

Test period 2011





Confirmed poor test performance

Summary of Results for TWIEX

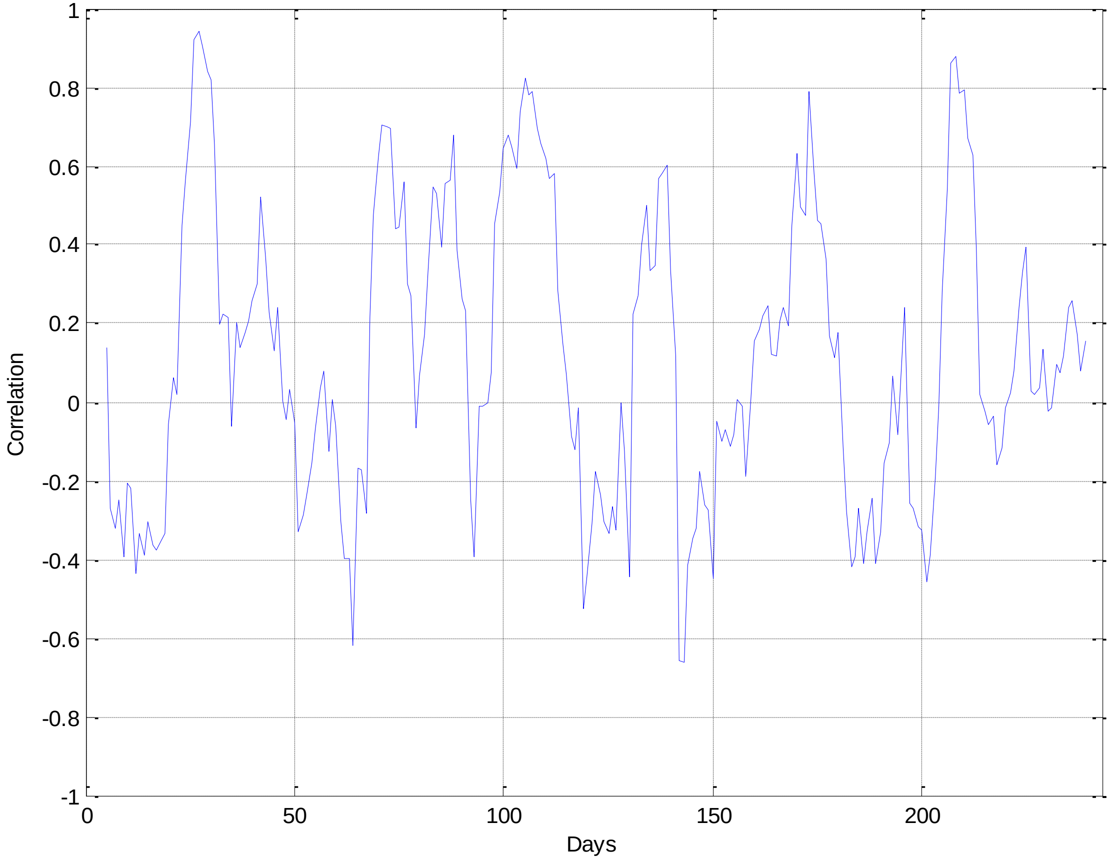
- *Market timing worked well* during past market conditions (i.e., 2004 – 2005 period)
- *Market timing does not work* under current market conditions (i.e., 2008 – 2012 period)
- Similar conclusions hold for

  - other international mutual funds

  - other time periods (say prior to 2004)

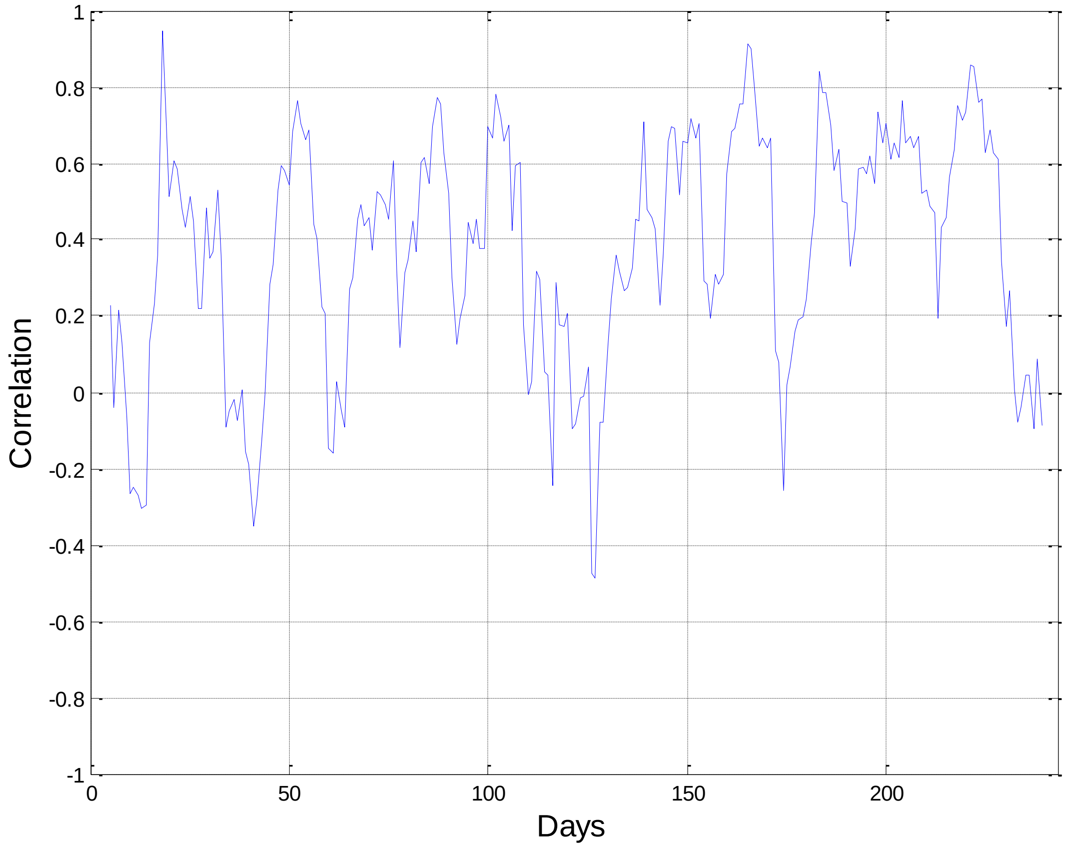
- **Explanation**: statistical characteristics of the stock market *have changed*

Correlation SP500-EURUSD year 2004 = 0.090



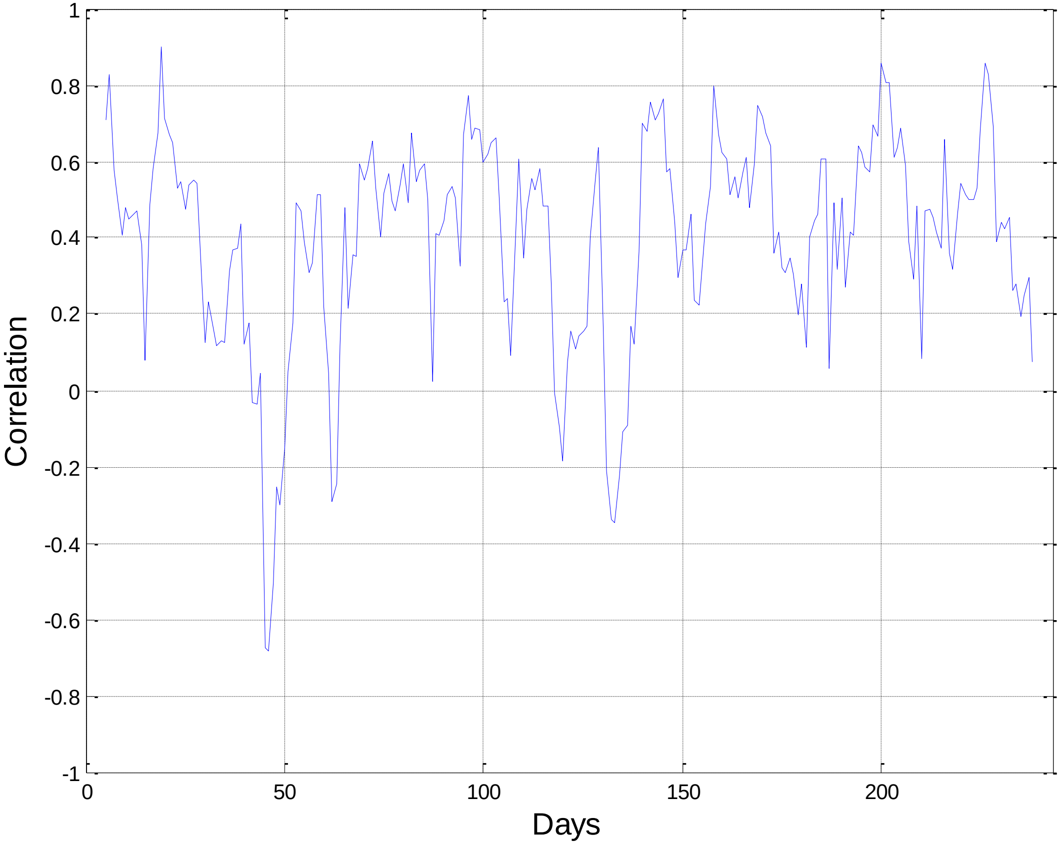
Correlation trend between SP500 and EURUSD for 2004 using a window of 9 days

Correlation SP500-EURUSD year 2010=0.394



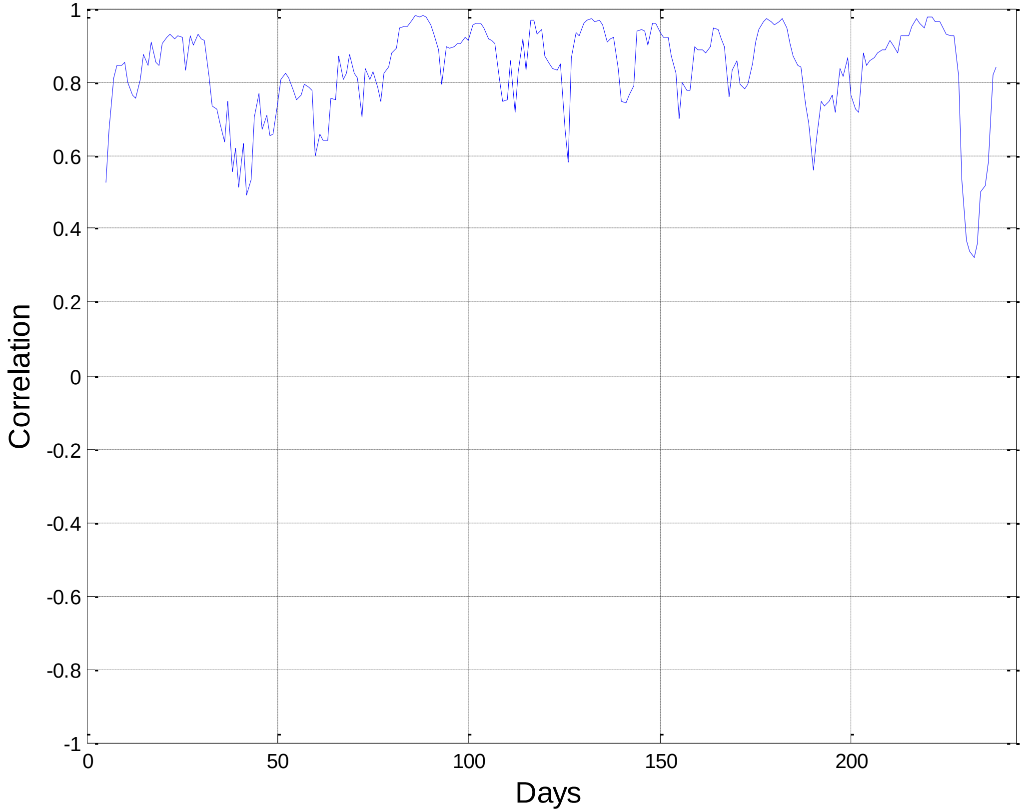
Correlation trend between SP500 and EURUSD for 2010 using a window of 9 days

Correlation SP500-TWIEX year 2005 = 0.429



Correlation trend between SP500 and TWIEX for 2005 using a window of 9 days

Correlation SP500-TWIEX year 2010 = 0.877



Correlation trend between SP500 and TWIEX for 2010 using a window of 9 days

Some possible interpretations

- International markets are more tightly linked (correlated) to US stock market, due to globalization and electronic trading.
- During 2009 – 2011 period, it is the US stock market that follows European markets (and not vice versa). – a large correlation btw SP500 & TWIEX.
- The procedure for calculating the daily NAV value of TWIEX has changed, in order to reflect more accurately the daily changes of the US stock market.

Aside: Interpretation vs Prediction

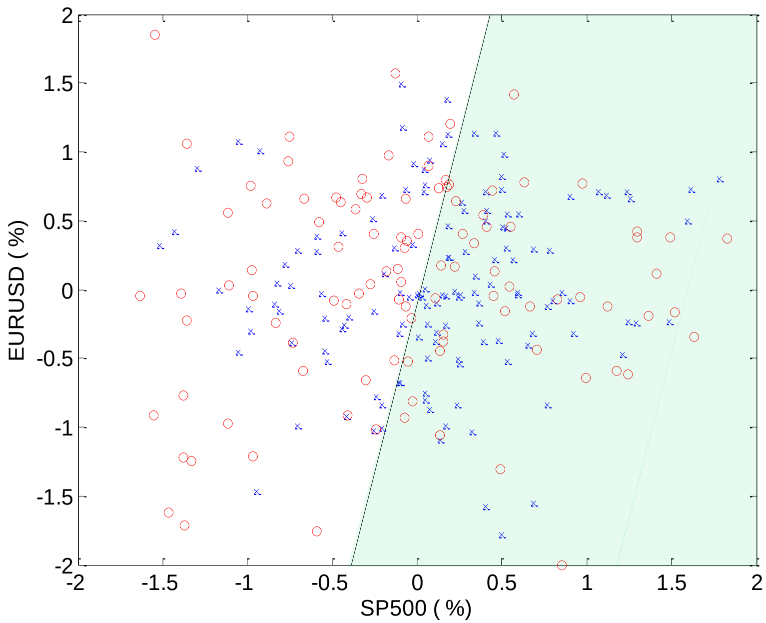
- Interpretation: outside the scope of VC-theory
- Only prediction can be *objectively evaluated*

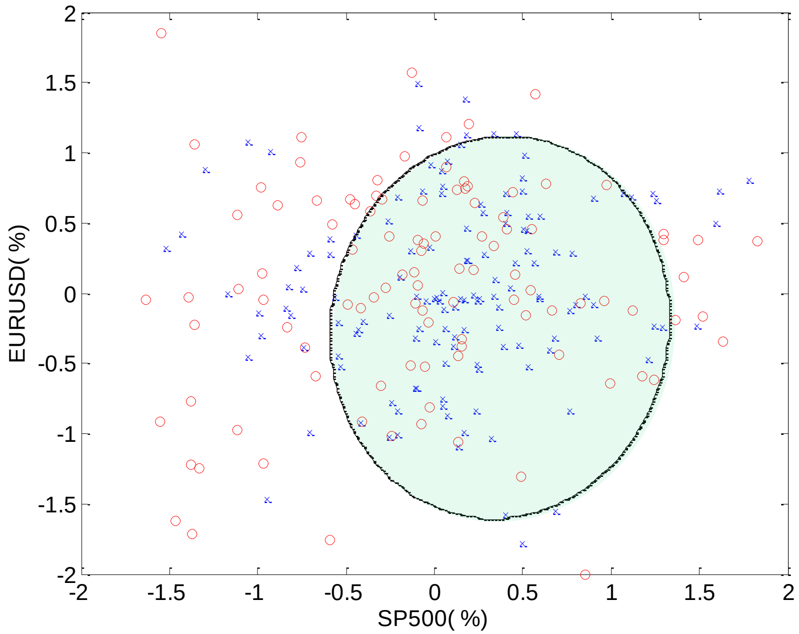
- **Multiplicity of good predictive models**, which reflect different aspects of the data
- *Which model is true?*

- Model interpretation should reflect application-domain knowledge, rather than data-analytic modeling alone

Interpretation vs Prediction

- Two good trading strategies estimated from 2004 training data





- Both models predict well for test period 2005
- *Which model is true?*

Conclusions and Policy Implications

- **Market timing of international funds**

  - has been indeed profitable **in the past**

  - **does not work** under present market conditions

- **Restrictions on frequent trading**

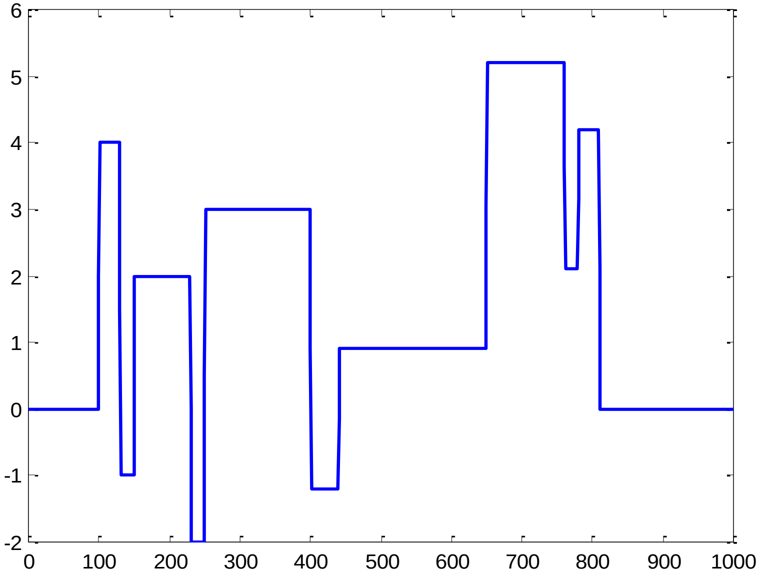
  - reflect past market conditions

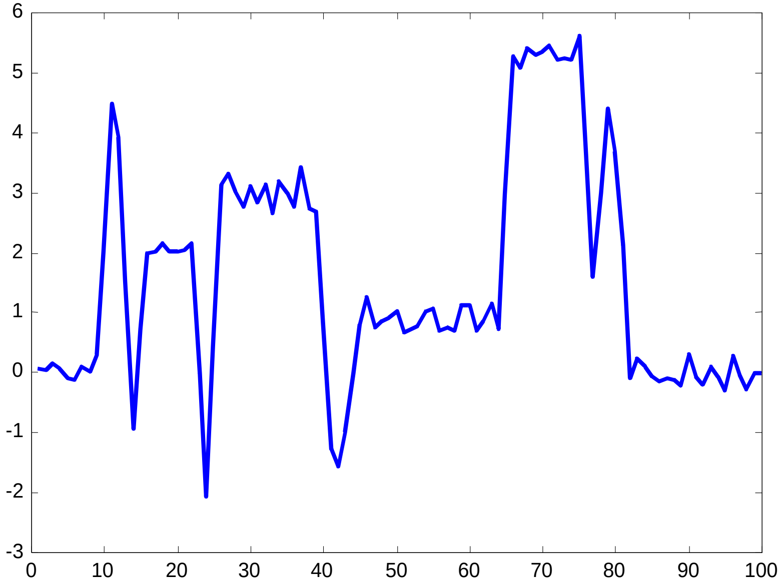
  - constrains risk management by small investors

- **Philosophical/policy question:**

  can these trading restrictions be really justified?

Application: signal denoising





Signal denoising problem statement

- **Regression formulation** ~ real-valued function estimation (with squared loss)
- **Signal representation**: linear combination of orthogonal basis functions (harmonic, wavelets)

$$y = \sum_i w_i g_i(x)$$

- **Differences** (from standard formulation)

  - fixed sampling rate

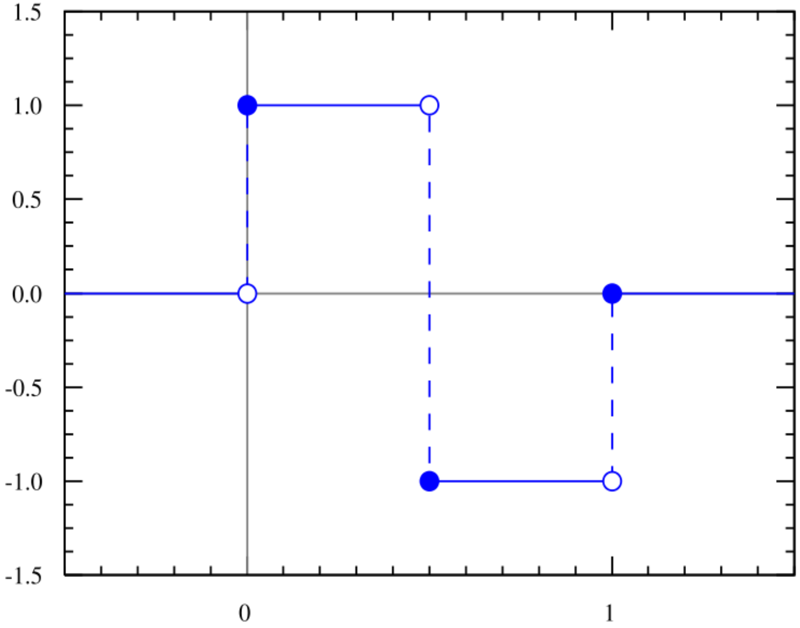
  - training data x-values = test data x-values

→ Computationally efficient orthogonal estimators: Discrete Fourier/Wavelet Transform (DFT / DWT)

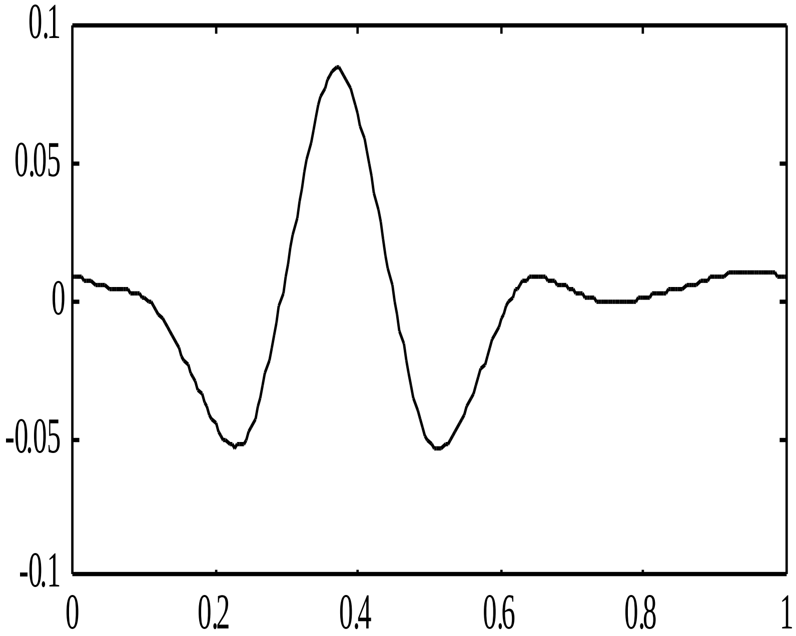
Examples of wavelets

see http://en.wikipedia.org/wiki/Wavelet

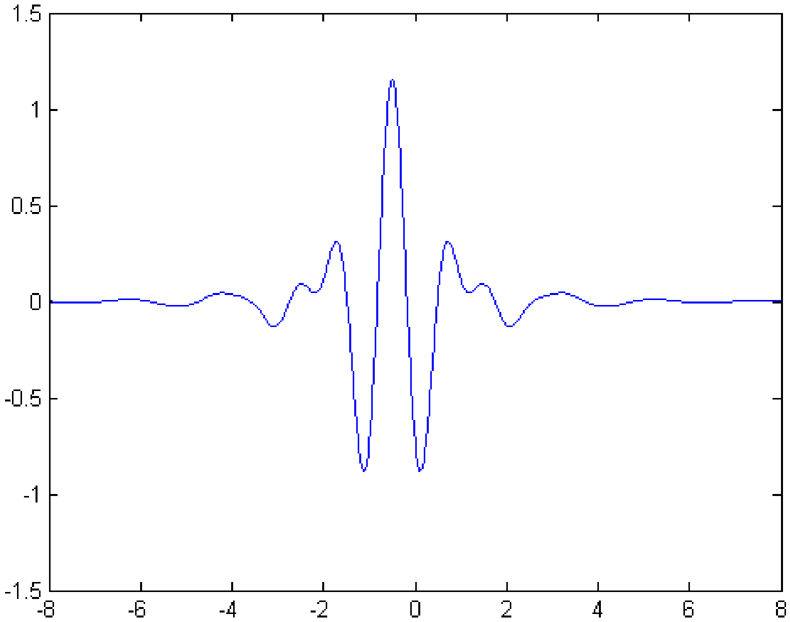
Haar wavelet



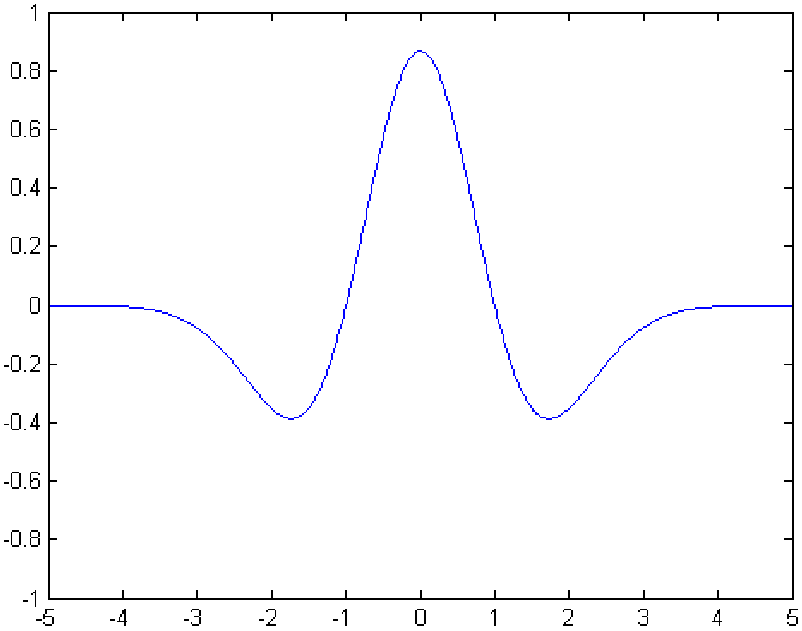
Symmlet



Meyer

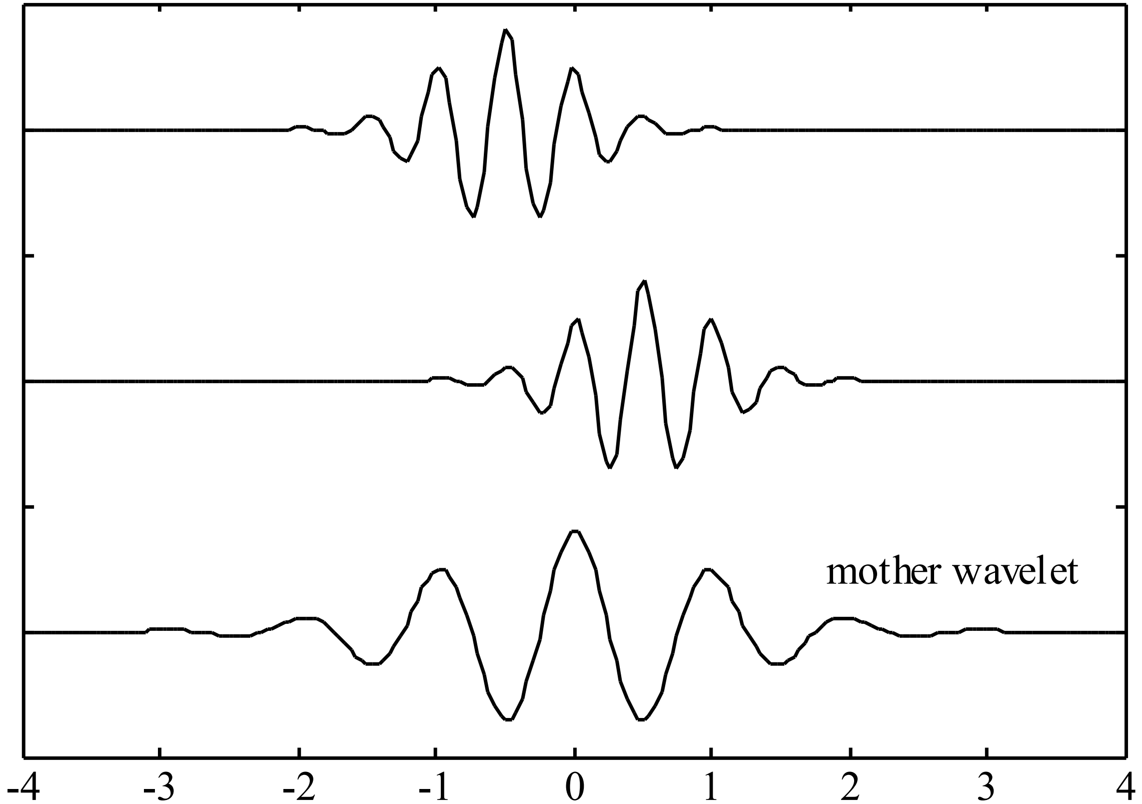


Mexican Hat



Wavelets (cont'd)

Example of translated and dilated wavelet basis functions:



Issues for signal denoising

- **Denoising via (wavelet) thresholding**
  - wavelet thresholding = sparse feature selection
  - nonlinear estimator suitable for ERM

- **Main factors for signal denoising** $y = \sum_i w_i g_i(x)$
  Representation (choice of basis functions)
  Ordering (of basis functions) ~ SRM structure
  Thresholding (~ model selection)
- **Large-sample setting**: representation
- **Finite-sample setting**: thresholding + ordering

VC framework for signal denoising

- **Ordering of (wavelet) thresholding =**

  = structure on orthogonal basis functions

  Traditional ordering $|w_{k1}| \geq |w_{k2}| \geq \ldots |w_{km}| \geq \ldots$

  Better ordering $\dfrac{|w_{k1}|}{freq_{k1}} \geq \dfrac{|w_{k2}|}{freq_{k2}} \geq \ldots \dfrac{|w_{km}|}{freq_{km}} \geq \ldots$

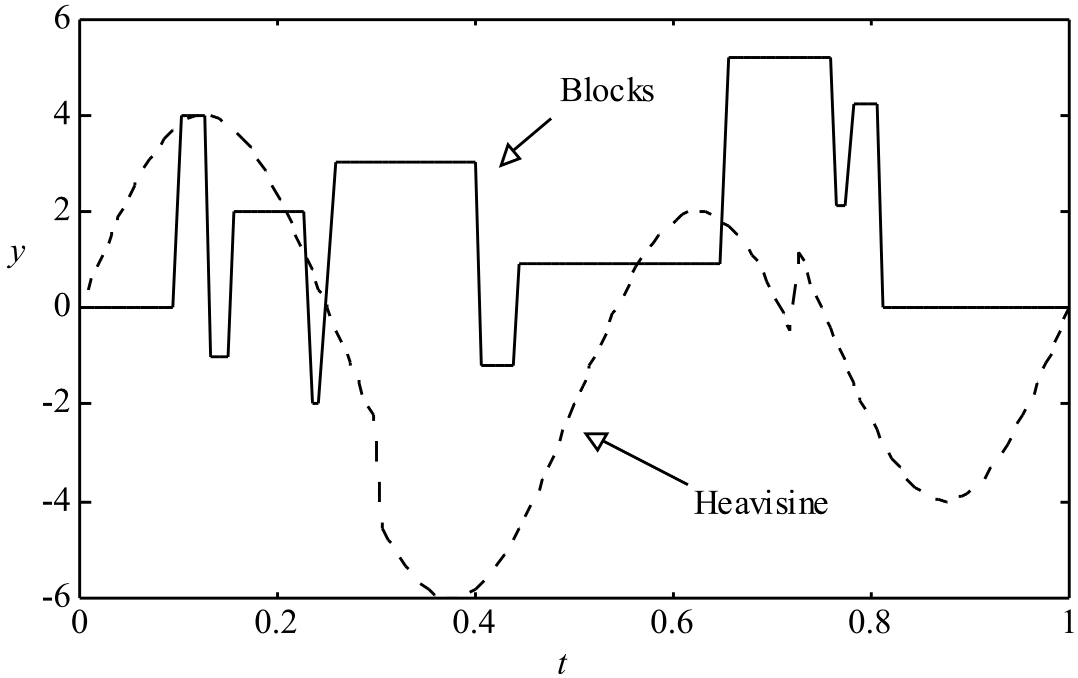
- **VC- thresholding**

  Opt number of wavelets ~ min of VC-bound

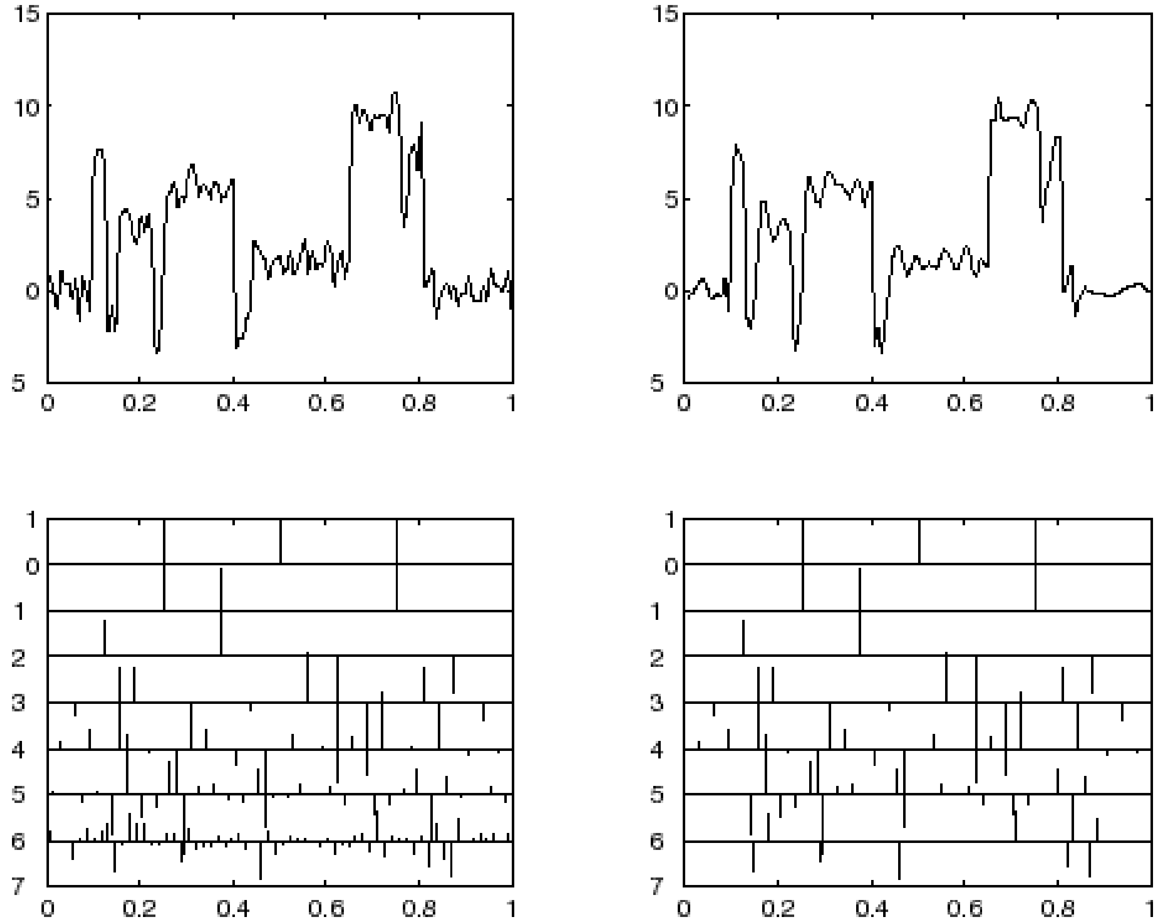
  Usually take VC-dim. *h=m* (number of wavelets or DoF)

Empirical Results: signal denoising

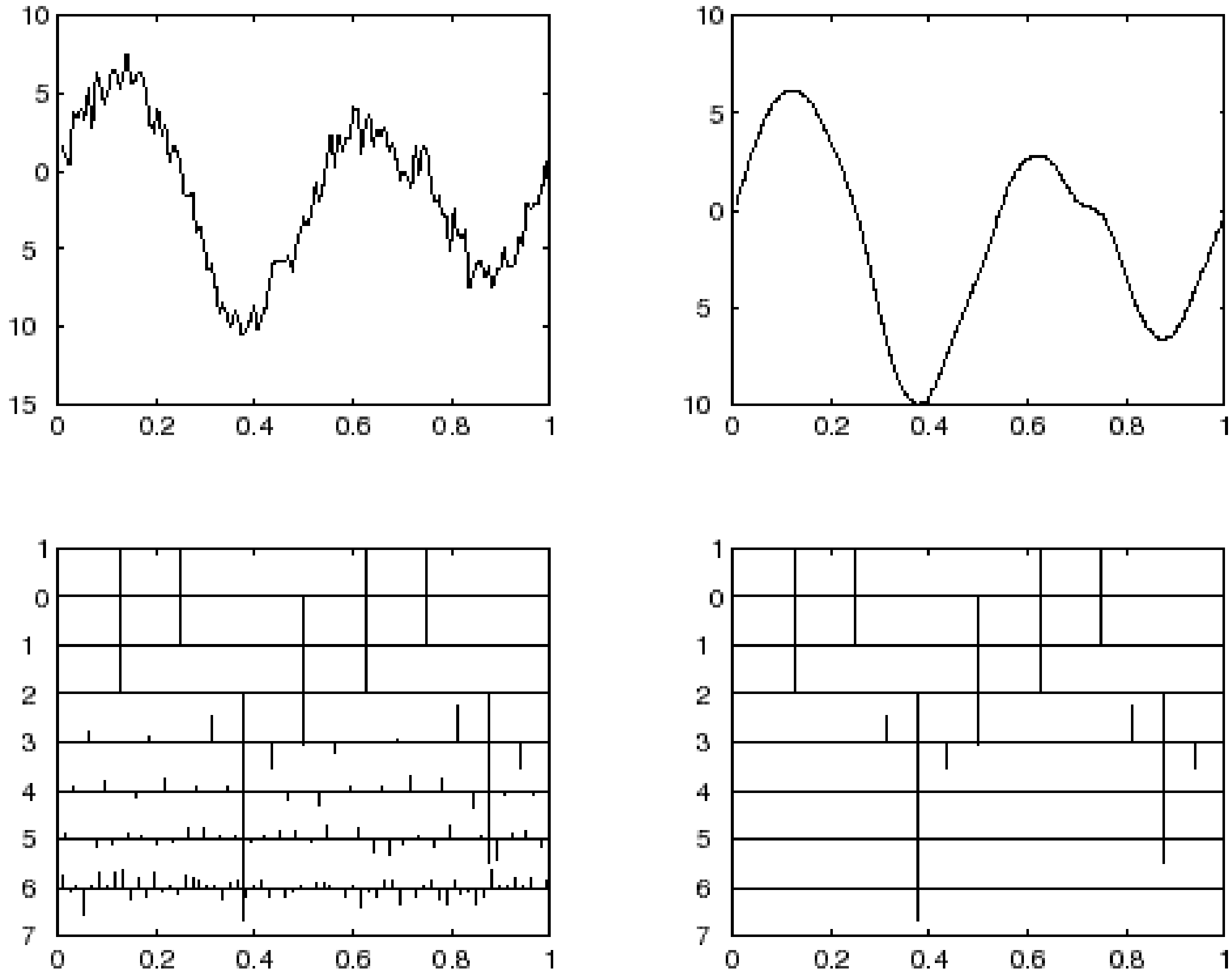
- **Two target functions**
- **Data set**: 128 noisy samples, SNR = 2.5



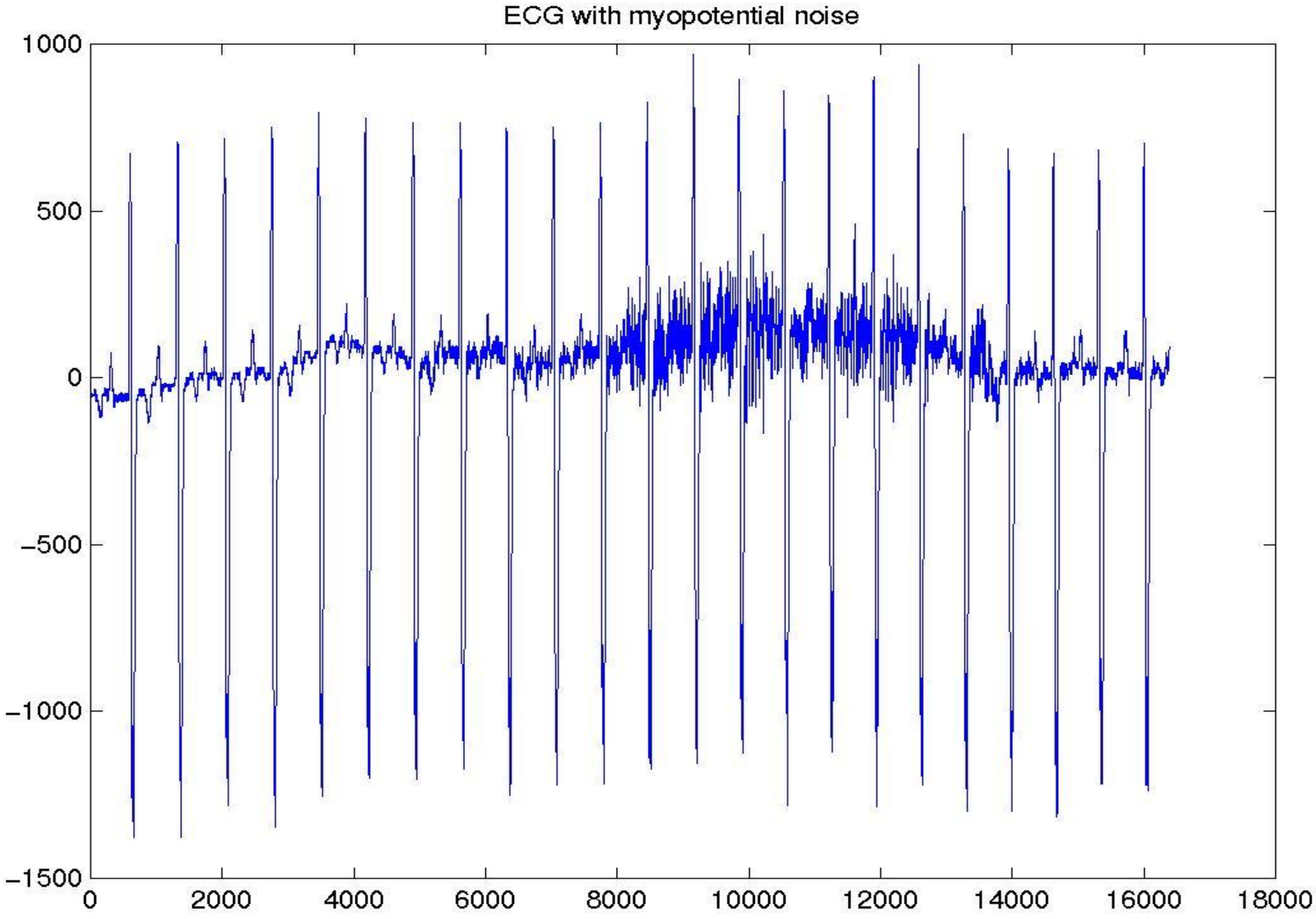
Empirical Results: Blocks signal estimated by VC-based denoising



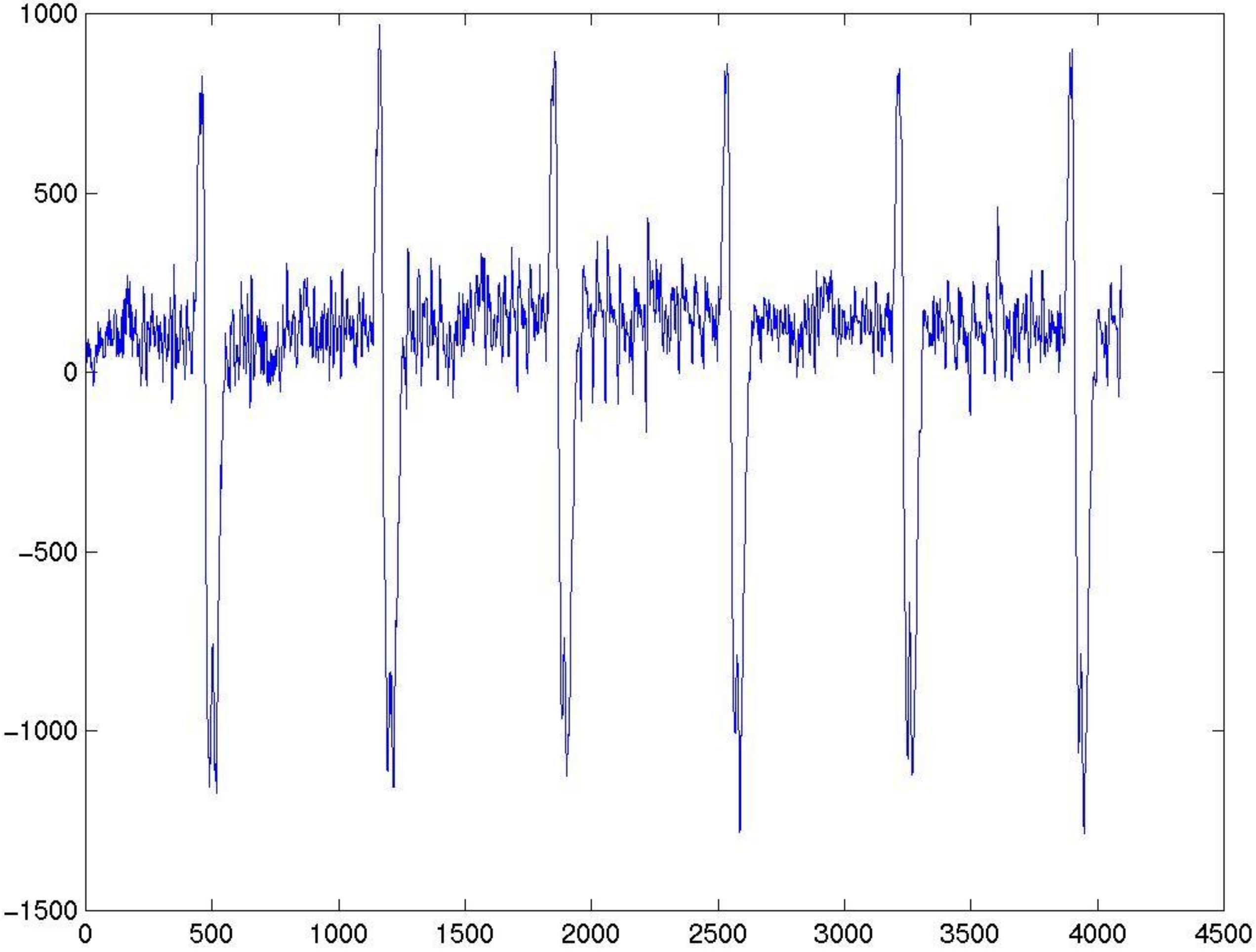
Empirical Results: Heavisine estimated by VC-based denoising



Application Study: ECG Denoising

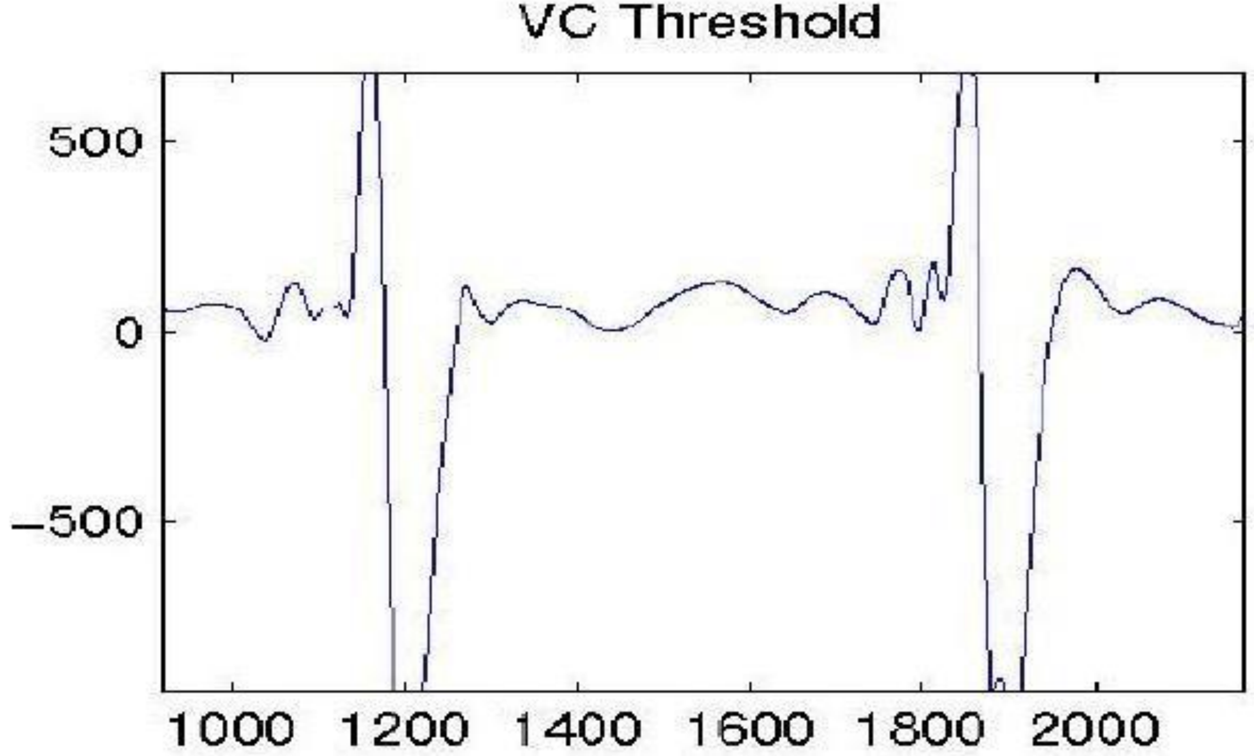


A closer look of a noisy segment



Denoised ECG signal

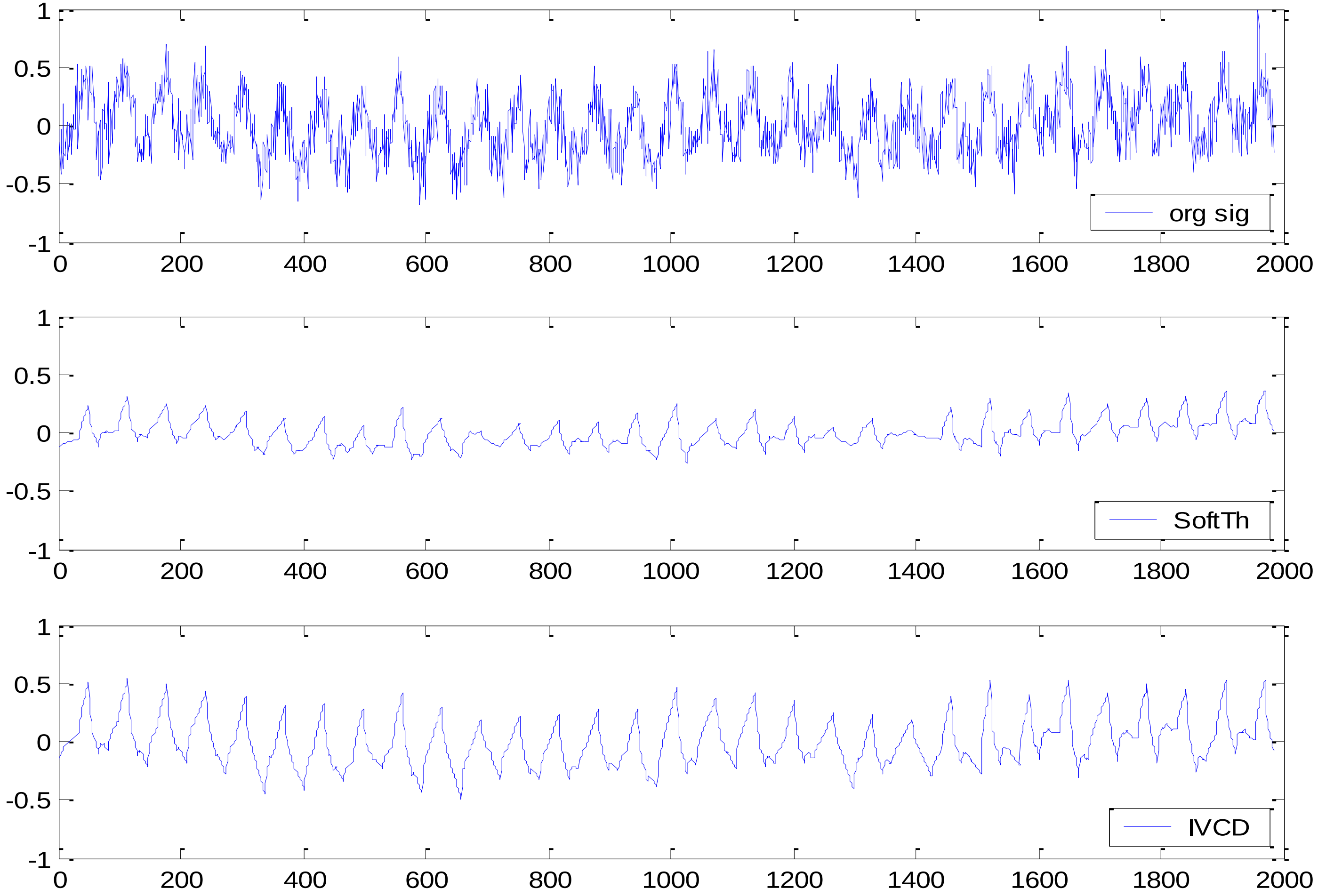
VC denoising applied to 4,096 noisy samples.
The final model (below) has 76 wavelets



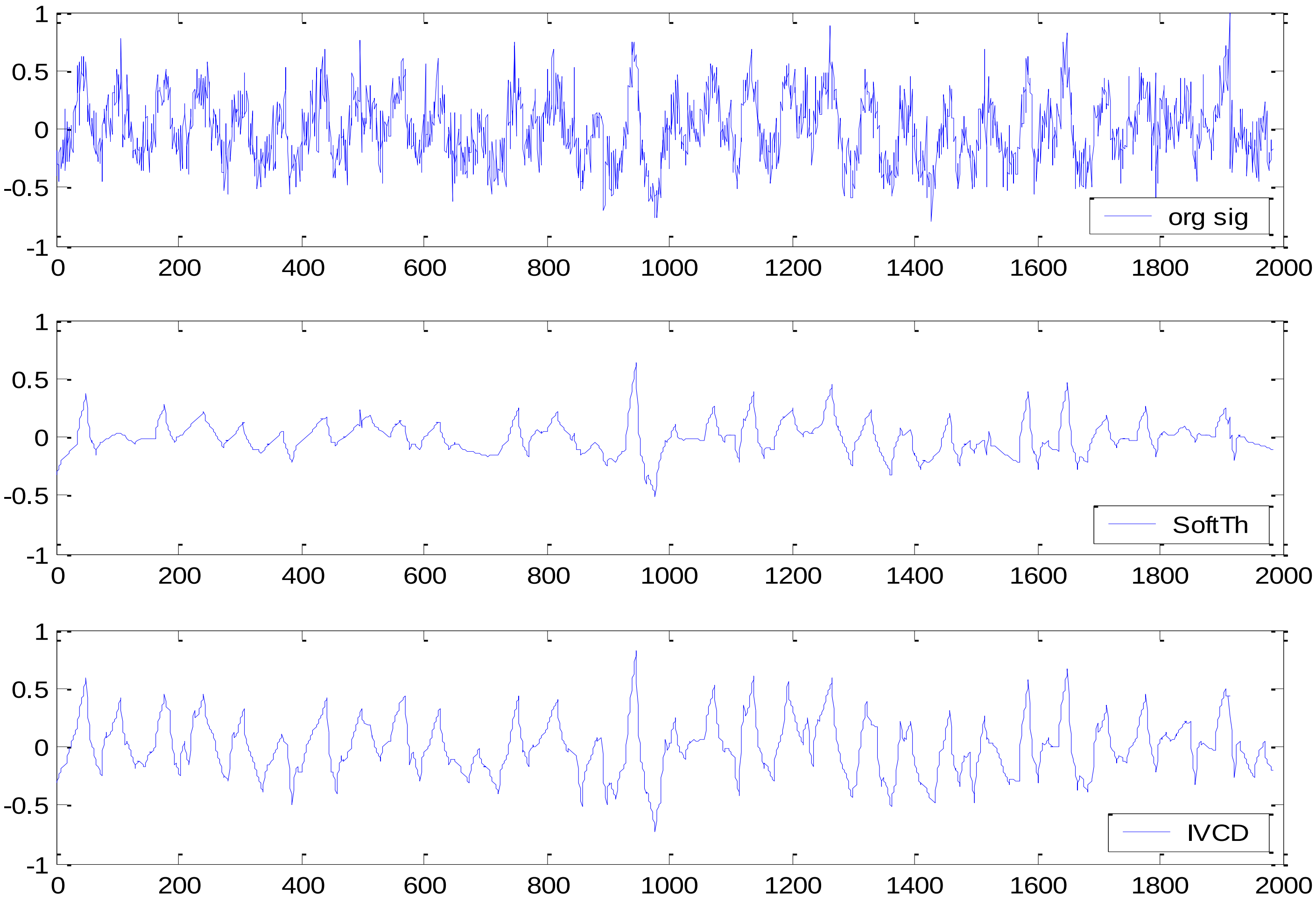
Application: fMRI signal denoising

- **MOTIVATION: understanding brain function via functional MRI**
- **DATA SET: provided by CMRR at UMN**
- **Signals (~ waveforms) recorded at a certain brain location response to external stimulus applied 32 times**
- ***Data Set 1*** **~ signals at the** ***visual cortex*** **in response to visual input light blinking 32 times**
- ***Data Set 2*** **~ signals at the** ***motor cortex*** **recorded when human subject moves his finger 32 times**
- **FMRI denoising = obtaining a better version of noisy signal**

Visual Cortex Data + Denoising



Motor Cortex Data + Denoising



Discussion

- **Application of VC-theory to signal denoising**
  - orthogonal basis functions
  - nonlinear estimator: sparse feature selection

- **Finite sample setting: importance of**
  - Ordering (of basis functions) ~ SRM structure
  - Model selection (thresholding)
- **Large-sample setting**:
  - type of basis functions (representation)

OUTLINE

- Objectives
- Inductive learning problem setting
- Statistical Learning Theory
- Applications
- **Measuring the VC-dimension**
- Summary and discussion

Measuring the VC-Dimension

- VC-dimension is difficult to estimate (for most practical learning methods)
- **Experimental estimation** (Vapnik et al1994) for binary classification problems
- **Main idea:**

  \- apply learning method to randomly labeled data and measure the training error

  \- the deviation of the training error from 0.5 depends on the flexibility (VC-dimension) of an estimator.

Measuring the VC-Dimension

- **Experimental estimation** (Vapnik et al1994) for binary classification problems:

  - Based on theoretic analysis of the maximum deviation of error rates between two independently labeled data sets

  - Perform repeated random experiments with different data sets and sample sizes

  - Estimate VC-dim by fitting the theoretic function (which depends only on *n/h*)

Measuring the VC-dim: Theory

- Consider binary classification, and denote *n* labeled training samples $\mathbf{Z}_n = \{\mathbf{z}_i, i = 1,..., n\}$
- Apply an estimator (learning method) to training data and measure the max deviation of error rates observed on two independently labeled data sets (of size *n*):

$$\xi(n) = \max_{\omega}(| Error(\mathbf{Z}_n^1) - Error(\mathbf{Z}_n^2) |)$$

- According to VC-theory, this deviation is bounded by

$$\xi(n) \le \Phi(n/h) \quad \text{or} \quad \xi(n) \approx \Phi(n/h)$$

where

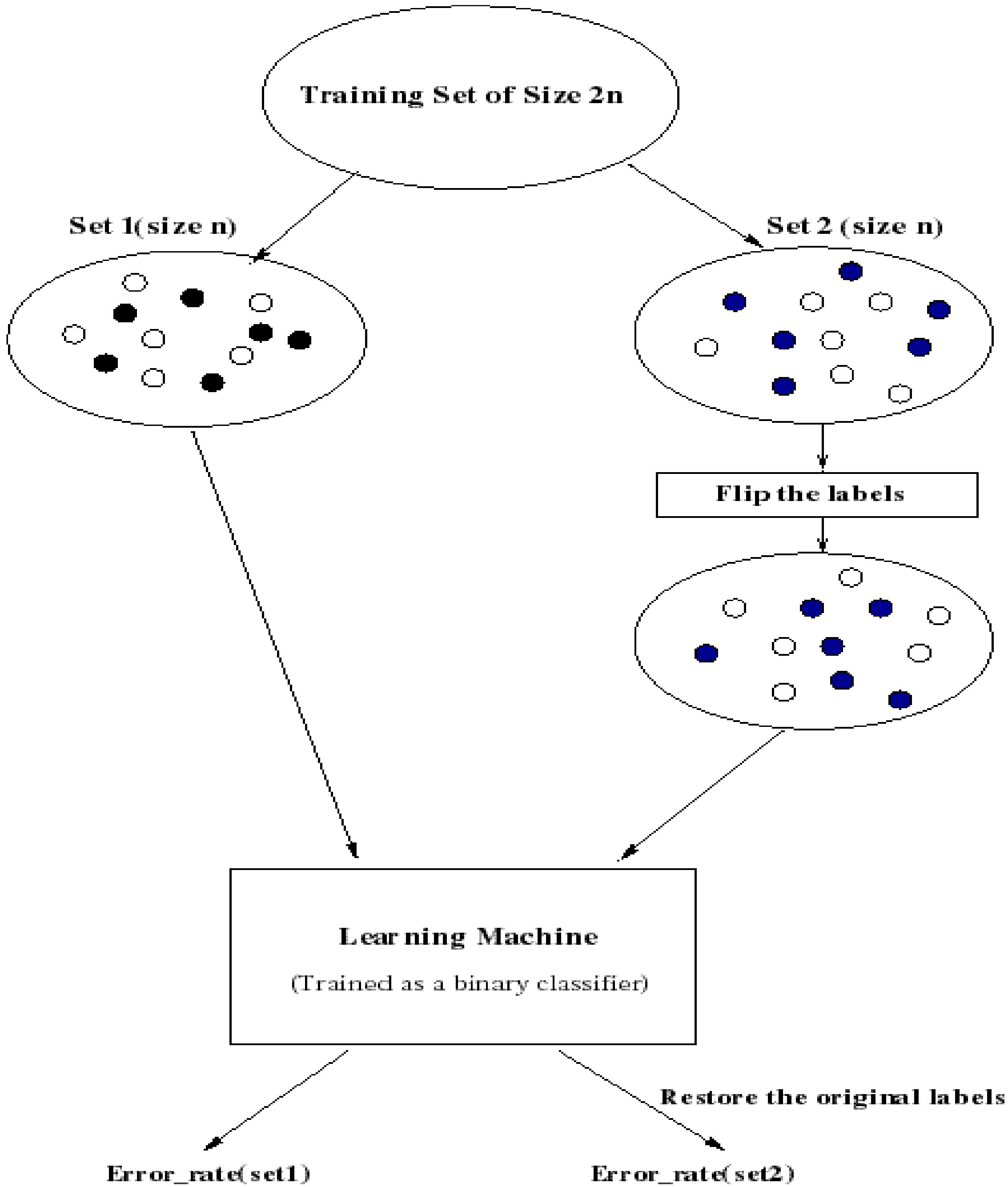
$$\Phi(\tau) = \begin{cases} 1 & if\,(\tau < 0.5) \\ a\dfrac{\ln(2\tau)+1}{\tau - k}\left(\sqrt{1 + \dfrac{b(\tau - k)}{\ln(2\tau)+1}} + 1\right) & otherwise \end{cases}$$

Measuring the VC-Dimension

Using experimental measurements of $\xi(n)$ we can fit these measurements to analytic function $\Phi(n/h)$ that depends only on VC-dim.

Experimental procedure (for one measurement)

- Generate a randomly labeled set of size *2n*
- Split it into two sets of equal size: Z1 and Z2
- Flip the class labels for the second set Z2
- Merge the two sets and train binary classifier
- Separate the sets and flip the labels on the second set back again
- Measure the difference between the error rates on the two sets: $\xi(n) = |Error(Z1)-Error(Z2)|$.


Training Set of Size 2n
Set 1(size n)
Set 2 (size n)
Flip the labels
Learning Machine
(Trained as a binary classifier)
Restore the original labels
Error_rate(set1)
Error_rate(set2)

Measuring the VC-Dimension

- Single measurements of $\xi(n)$ is affected by random variability of random sample
- To reduce variability:

  - the experiment is repeated for different data sets with varying sample sizes $n_1, n_2, \dots, n_k$, in the range $0.5 \leq n_i/h \leq 30$

  - several (m_i) repeated experiments are performed for each sample size n_i
- The effective VC-dimension provides the best fit between $\Phi(n/h)$ and measured values $\bar{\xi}(n_i)$

$$h^* = \arg\min_h \sum_{i=1}^{k} [\bar{\xi}(n_i) - \Phi(n_i / h)]^2$$

Measuring the VC-Dimension

- Can be applied to estimating the VC-dimension of penalized estimators (ridge regression), i.e. finding dependency *h=h(lambda)*
  - see Example 7.1 on p.266 (in the textbook)

- This dependency can be then used for *analytic model selection* using practical VC-bound
- Empirical results show that estimated VC-dimension works better than using ‘effective’ DoF for ridge regression, in conjunction with analytic model selection criteria.

OUTLINE

- Objectives
- Inductive learning problem setting
- Statistical Learning Theory
- Applications
- Measuring the VC-dimension
- **Summary and discussion**

Summary and Discussion: VC-theory

- **Methodology**
  - learning problem setting (KID principle)
  - concepts (risk minimization, VC-dim., structure)
- **Interpretation/ evaluation of existing methods**
- **Model selection** using VC-bounds
- **Basis for new types of inference** (TBD later)
- **Clear limitations/constraints** for all learning methods based on the idea of ERM
- **What a theory cannot do**:
  - provide formalization (for a given application)
  - select 'good' structure (for a given application)
  - always a gap between theory and applications

References

- **General references on VC-theory**

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