Least Squares Support Vector Regression with Applications to Large-Scale Data: a Statistical Approach

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Co-Promotor: Prof. dr. ir. J. Suykens

Outline

1. Goal & Overview
2. Introduction
   - Parametric vs. nonparametric regression
   - Nonparametric regression estimates: an overview
3. Fixed-Size Least Squares Support Vector Machines
   - Fixed Size LS-SVM formulation
   - Selection of Support Vectors
   - Practical identification problem
4. Robust Nonparametric Methods
   - Problems with outliers
   - Robust nonparametric regression
5. Correlated Errors
   - Problems with correlation in nonparametric regression
   - Removing correlation effects
6. Confidence Intervals
7. Conclusions

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Goal of the Thesis

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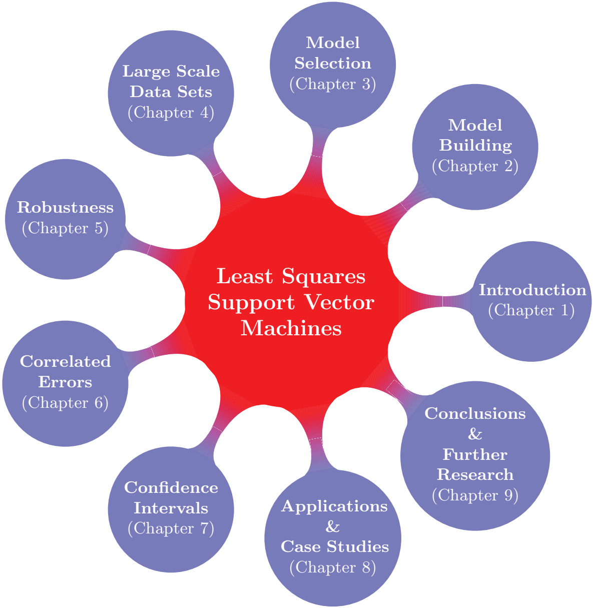
Study the properties of Least Squares Support Vector Machines for regression with an emphasis on statistical aspects and develop a framework for large scale data

Overview


Least Squares Support Vector Machines
Introduction (Chapter 1)
Model Building (Chapter 2)
Model Selection (Chapter 3)
Large Scale Data Sets (Chapter 4)
Robustness (Chapter 5)
Correlated Errors (Chapter 6)
Confidence Intervals (Chapter 7)
Applications & Case Studies (Chapter 8)
Conclusions & Further Research (Chapter 9)

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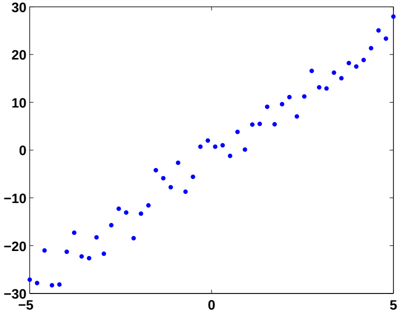
A simple example



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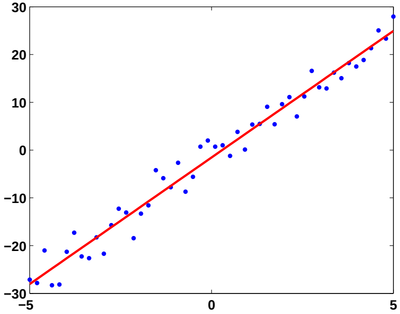

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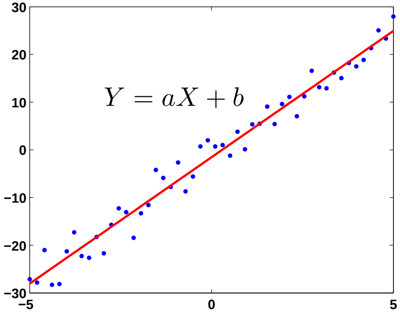

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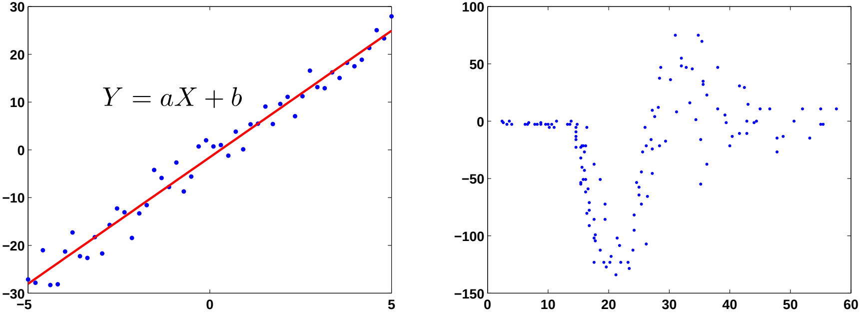

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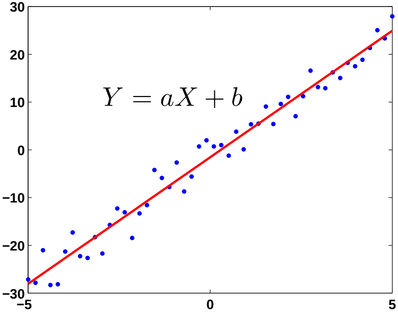

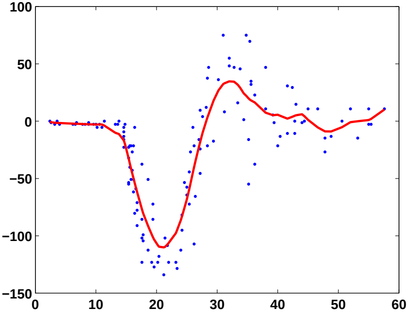

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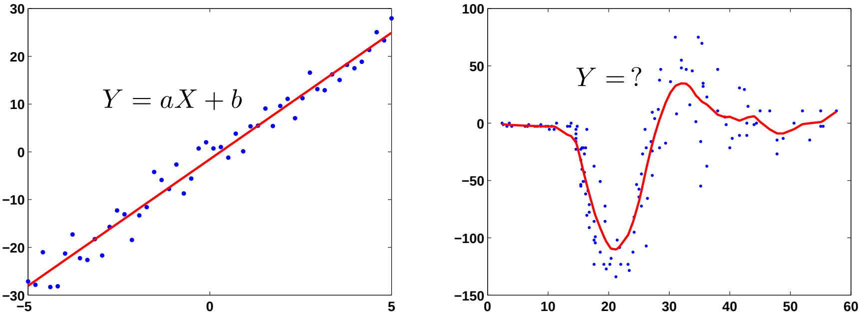

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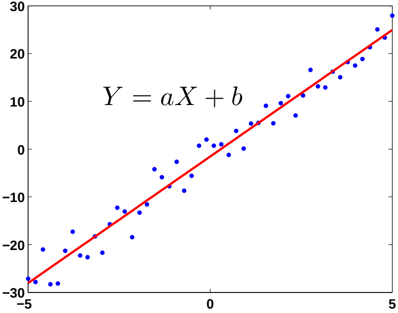
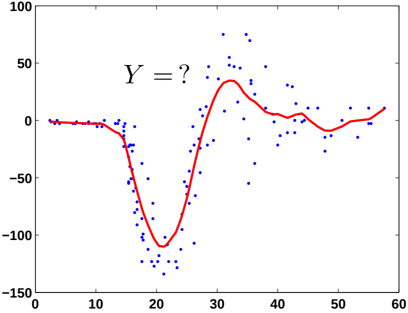
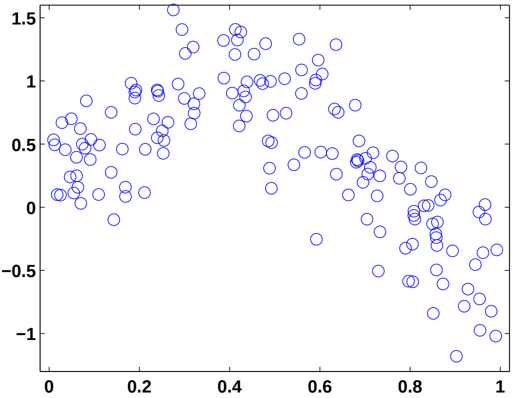




PARAMETRIC FORM IS NOT ALWAYS EASY TO FIND

Construction of a nonparametric estimate: NW smoother



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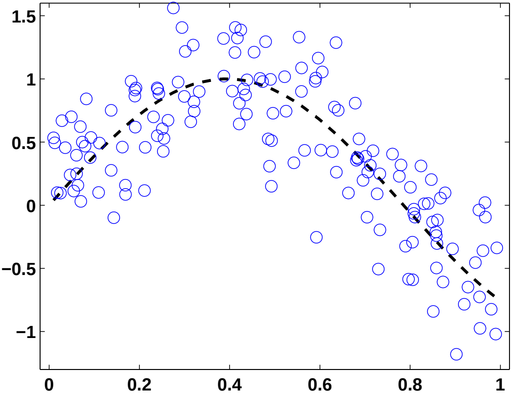

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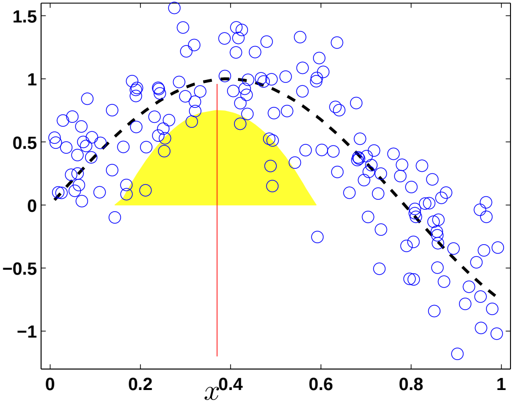

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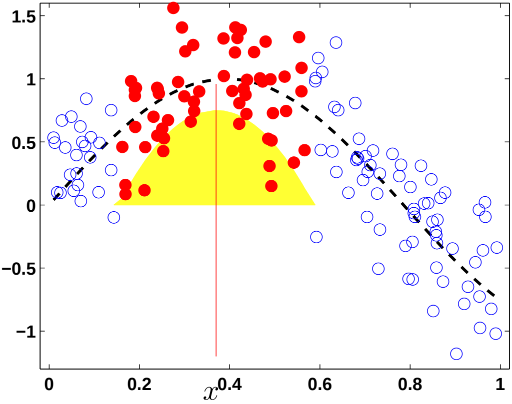

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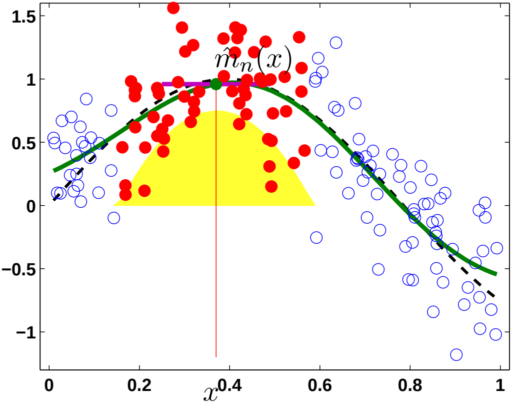

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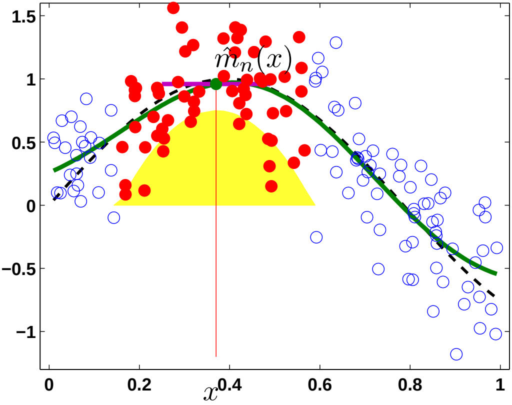

$$\hat{m}_n(x) = \sum_{i=1}^{n} \frac{K(\frac{x-X_i}{h})}{\sum_{j=1}^{n} K(\frac{x-X_j}{h})} Y_i$$

Other nonparametric regression estimates

- Local constant regression (Nadaraya, 1964; Watson, 1964)
- Regression trees (Breiman *et al.*, 1984)
- Wavelets (Daubechies, 1992)
- Nearest Neighbors (Devroye *et al.*, 1994)
- Local linear regression (Fan & Gijbels, 1996)
- Support vector machines (Vapnik, 1995)
- Splines (Wahba, 1990; Eubank, 1999)
- Partitioning estimates (Györfi *et al.*, 2002)
- **Least squares support vector machines** (Suykens *et al.*, 2002)
- ...

Least squares support vector machines

Primal formulation (LS-SVM formulation for regression)

$$\min_{w,b,e} \mathcal{J}_P(w,e) = \tfrac{1}{2} w^T w + \tfrac{\gamma}{2} \textstyle\sum_{k=1}^{n} e_k^2$$
$$s.t. \quad w^T \varphi(X_k) + b + e_k = Y_k, \quad k = 1, \ldots, n.$$

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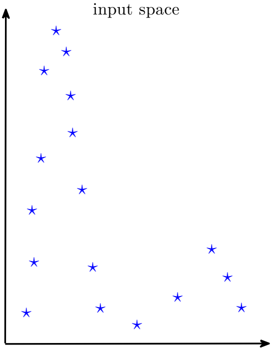

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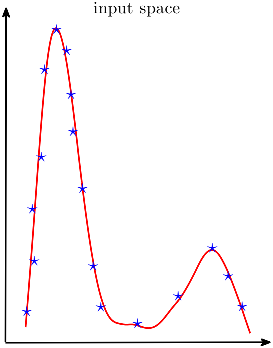

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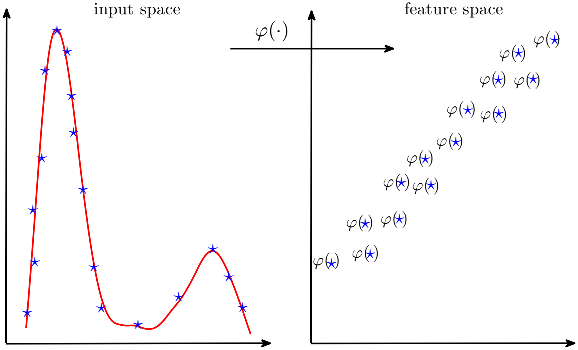

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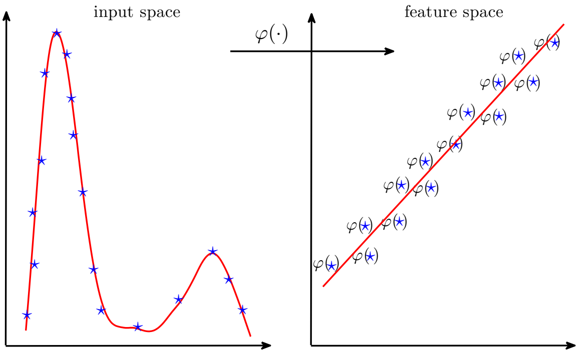


LS-SVM: solution + model selection

- $\mathcal{D}_n = \{(X_k, Y_k) : X_k \in \mathbb{R}^d, Y_k \in \mathbb{R}; k = 1, \ldots, n\} \overset{\text{i.i.d.}}{\sim} (X, Y)$

Primal formulation

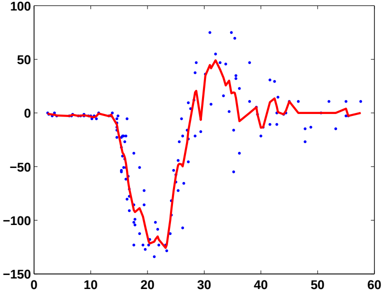
$$\min_{w,b,e} \mathcal{J}_P(w, e) = \frac{1}{2} w^T w + \frac{\gamma}{2} \sum_{k=1}^{n} e_k^2$$
$$s.t. \quad Y_k = w^T \varphi(X_k) + b + e_k, \quad k = 1, \ldots, n.$$

Dual formulation

$$\left(\begin{array}{c|c} 0 & 1_n^T \\ \hline 1_n & \Omega + \frac{I_n}{\gamma} \end{array}\right) \left(\begin{array}{c} b \\ \hline \alpha \end{array}\right) = \left(\begin{array}{c} 0 \\ \hline Y \end{array}\right)$$

- $\Omega_{kl} = \varphi(X_k)^T \varphi(X_l) = K(X_k, X_l) = (2\pi)^{-d/2} \exp(-\frac{\|X_k - X_l\|^2}{2\mathbf{h}^2})$
- K has to be positive definite i.e. $\int \exp(-j\omega x) K(x)\, dx \geq 0$
- Model in dual space $\hat{m}_n(x) = \sum_{k=1}^{n} \hat{\alpha}_k K(x, X_k) + \hat{b}$
- γ and $\mathbf{h}$: tuning parameters $\Rightarrow$ **cross-validation**

Effect of the tuning parameters



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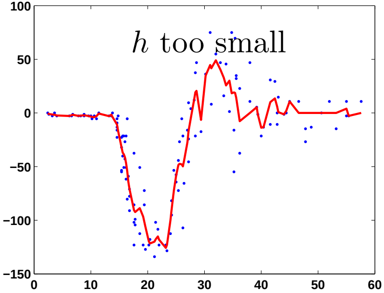

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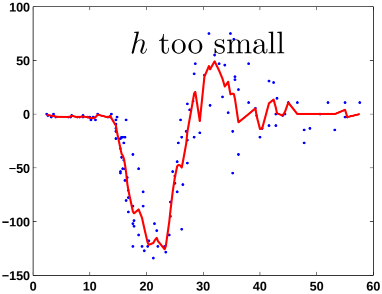

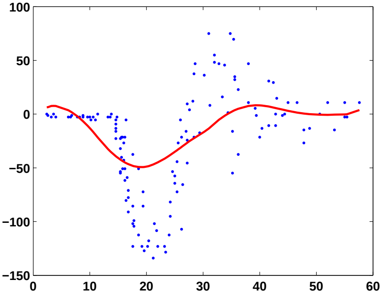

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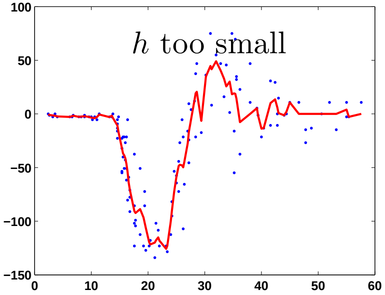

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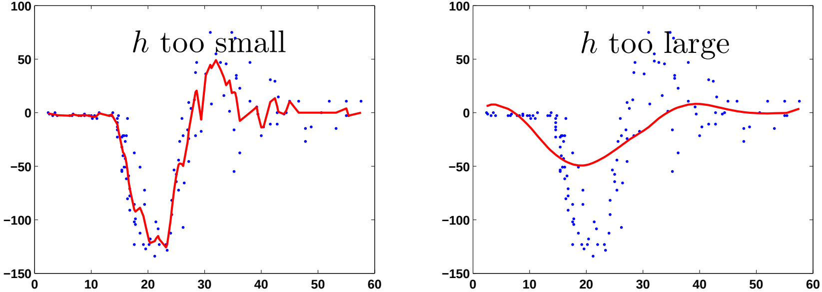

Model selection criteria are ABSOLUTELY needed

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Estimation in Primal Space

- LS-SVM formulation for regression

Primal formulation

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$$s.t. \quad w^T\varphi(X_k) + b + e_k = Y_k, \quad k = 1,\ldots,n.$$

- Can we solve the LS-SVM in primal space instead of dual?
- Approximation of feature map φ needed
- Is it possible to compute such a mapping?
  - φ can be infinite dimensional
  - Solution:use a *fixed size* m of support vectors to approximate φ
  - Solve the above as primal ridge regression

Problems with Large Scale Data

1. Calculation and/or storage kernel matrix Ω
   - $N = 1.000 \Rightarrow \Omega \Rightarrow 8$ MB
   - $N = 10.000 \Rightarrow \Omega \Rightarrow 763$ MB
   - $N = 20.000 \Rightarrow \Omega \Rightarrow 3051$ MB
2. If possible to compute, how long would it take?

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2. If possible to compute, how long would it take?

$\Rightarrow$ Solution: Matrix Approximations (Nyström, 1930)

$$\hat{\varphi}_i(x) \overset{m \ll n}{\approx} \frac{\sqrt{m}}{\lambda_i^{(m)}} \sum_{k=1}^{m} K(X_k, x) u_{ki}^{(m)}$$

Fixed Size LS-SVM formulation

- Given: approximation to the feature map

Primal formulation

$$\min_{w,b,e} \mathcal{J}_P(w,e) = \frac{1}{2} w^T w + \frac{\gamma}{2} \sum_{k=1}^{n} e_k^2$$
$$s.t. \quad w^T \hat{\varphi}(X_k) + b + e_k = Y_k, \quad k = 1, \ldots, n.$$

- Solution

$$\begin{pmatrix} w \\ b \end{pmatrix} = \left(\hat{\Phi}_e^T \hat{\Phi}_e + \frac{I_{m+1}}{\gamma} \right)^{-1} \hat{\Phi}_e^T Y,$$

with

$$\hat{\Phi}_e = \begin{pmatrix} \hat{\varphi}_1(X_1) & \cdots & \hat{\varphi}_m(X_1) & 1 \\ \vdots & \ddots & \vdots & \vdots \\ \hat{\varphi}_1(X_n) & \cdots & \hat{\varphi}_m(X_n) & 1 \end{pmatrix}$$

Selection of support vectors: Rényi Entropy

- Maximize quadratic Rényi entropy: $H_{R2}^{m} = -\log \int f(x)^2 \, dx$

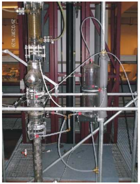
Theorem (Maximizing Entropy)

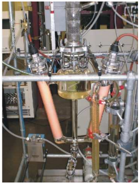
The Rényi entropy on a closed interval $[a, b]$ with $a, b \in \mathbb{R}$ and no additional moment constraints is maximized for the uniform density $1/(b-a)$.

(Selecting SV) (Wrong Bandwidth)

Identification of a pilot scale distillation column

- Joint work with Bart Huyck (CIT)





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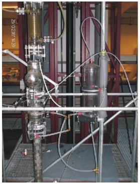

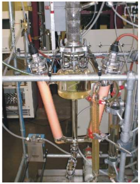

- Task: identify bottom temperature column with LS-SVM

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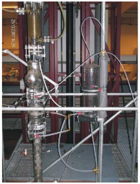

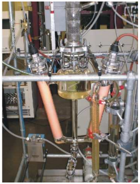

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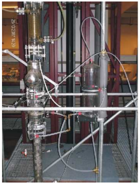

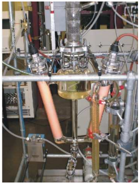

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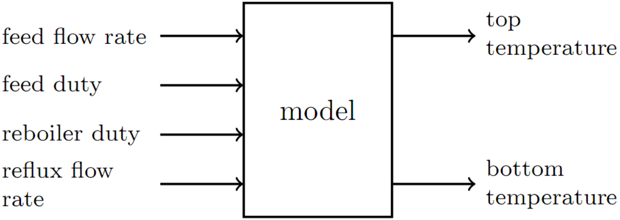

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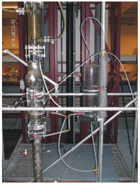

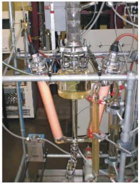

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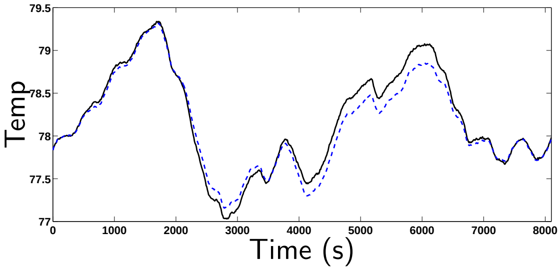

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Problems with outliers in parametric regression

- model: $Y_k = aX_k + b + e_k, \quad k = 1, \dots, n$
- (a, b) estimated from data
- LS principle: $(\hat{a}, \hat{b}) = \underset{a,b \in \mathbb{R}^2}{\arg\min} \frac{1}{n} \sum_{k=1}^{n} [Y_k - (aX_k + b)]^2$

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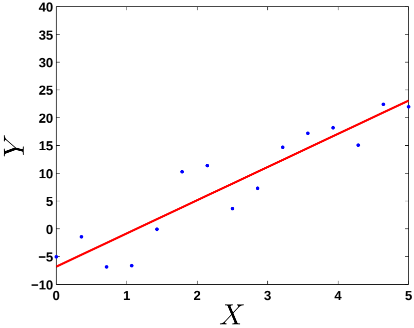

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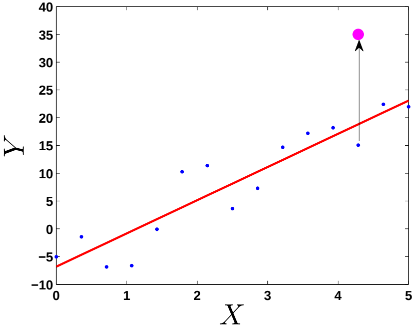

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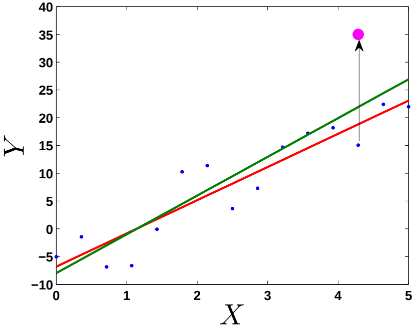
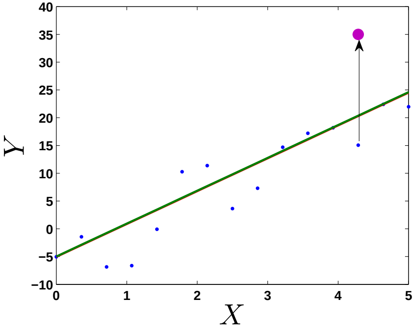


- LS principle is NOT robust

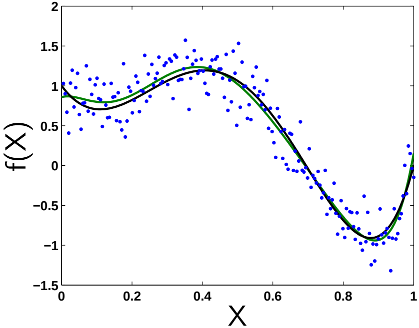
Problems with outliers in parametric regression

- model: $Y_k = aX_k + b + e_k, \quad k = 1, \ldots, n$
- (a, b) estimated from data
- LS principle: $(\hat{a}, \hat{b}) = \underset{a,b \in \mathbb{R}^2}{\arg\min} \frac{1}{n} \sum_{k=1}^{n} [Y_k - (aX_k + b)]^2$



- LS principle is NOT robust
- Solution LAD: $(\hat{a}, \hat{b}) = \underset{a,b \in \mathbb{R}^2}{\arg\min} \frac{1}{n} \sum_{k=1}^{n} |Y_k - (aX_k + b)|$

Problems with outliers in nonparametric regression



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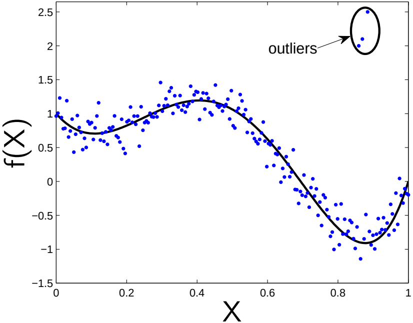

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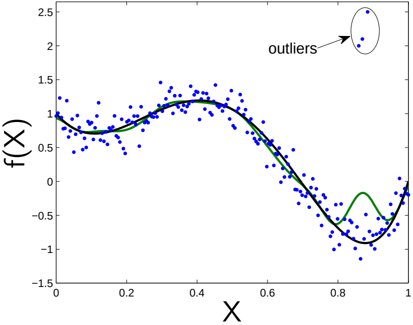

- LS principle ⇒ sensitive to outliers (and leverage points)
- Linear/polynomial kernel ⇒ non-robust methods
- Using appropriate CV ⇒ robust CV

Iterative Reweighting & Weight Functions

Primal formulation

$$\min_{w,b,e} \mathcal{J}_P(w,e) = \frac{1}{2}w^T w + \frac{\gamma}{2}\sum_{k=1}^{n} e_k^2$$
$$s.t. \quad Y_k = w^T \varphi(X_k) + b + e_k, \quad k = 1,\ldots,n.$$

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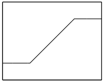
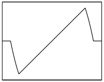
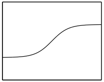
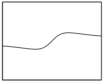
	Huber	Hampel	Logistic	Myriad
$V(r)$	$\begin{cases} 1, & \text{if } \lvert r\rvert < \beta; \\ \frac{\beta}{\lvert r\rvert}, & \text{if } \lvert r\rvert \geq \beta. \end{cases}$	$\begin{cases} 1, & \text{if } \lvert r\rvert < b_1; \\ \frac{b_2 - \lvert r\rvert}{b_2 - b_1}, & \text{if } b_1 \leq \lvert r\rvert \leq b_2; \\ 0, & \text{if } \lvert r\rvert > b_2. \end{cases}$	$\frac{\tanh(r)}{r}$	$\frac{\delta^2}{\delta^2 + r^2}$
$\psi(r)$				
$L(r)$	$\begin{cases} r^2, & \text{if } \lvert r\rvert < \beta; \\ \beta\lvert r\rvert - \frac{1}{2}\beta^2, & \text{if } \lvert r\rvert \geq \beta. \end{cases}$	$\begin{cases} r^2, & \text{if } \lvert r\rvert < b_1; \\ \frac{b_2 r^2 - \lvert r^3\rvert}{b_2 - b_1}, & \text{if } b_1 \leq \lvert r\rvert \leq b_2; \\ 0, & \text{if } \lvert r\rvert > b_2. \end{cases}$	$r\tanh(r)$	$\log(\delta^2 + r^2)$

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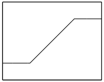
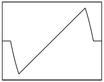
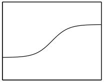
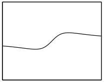
$\psi(r)$				
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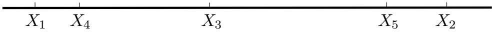

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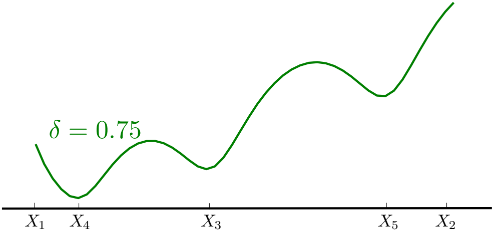

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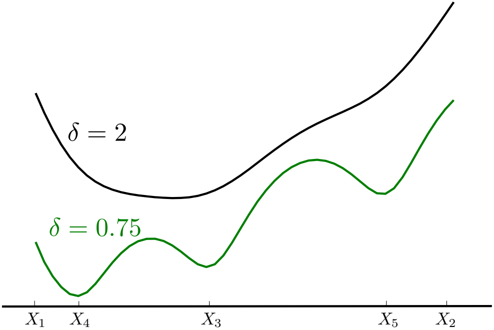

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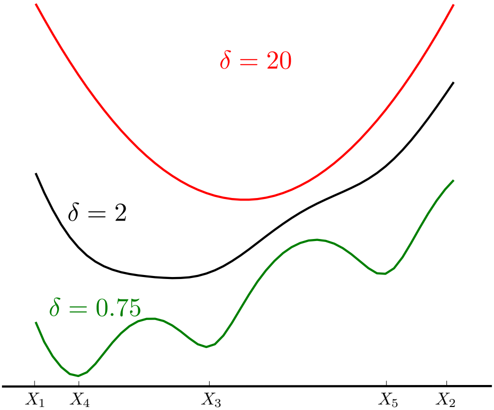

To obtain a fully robust solution...

- robust smoother
- bounded kernel
- robust CV $\Rightarrow L'$ bounded

$$RCV(\theta) = \frac{1}{n} \sum_{i=1}^{n} L\left(Y_i - \hat{m}_n^{(-i)}(X_i;\theta)\right)$$

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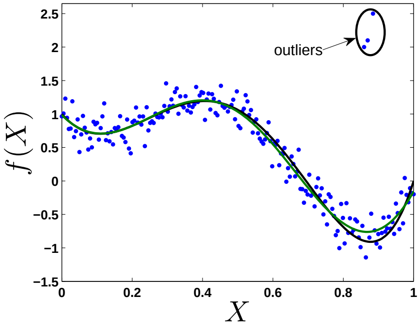

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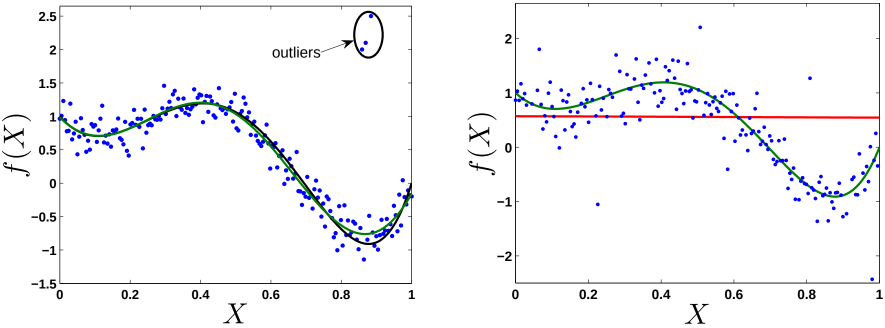

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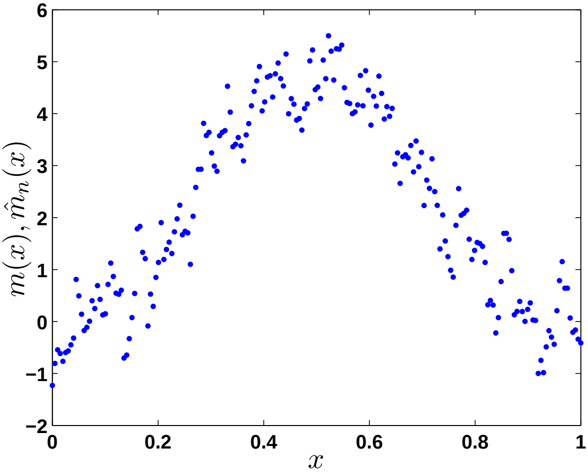

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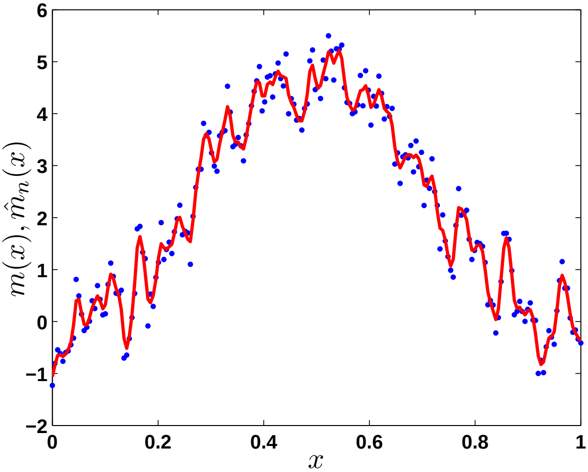

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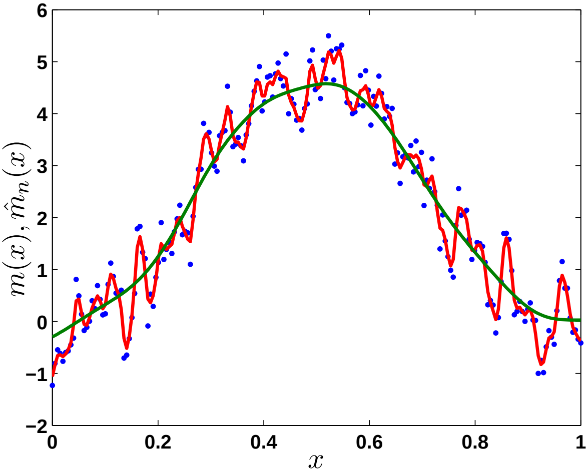

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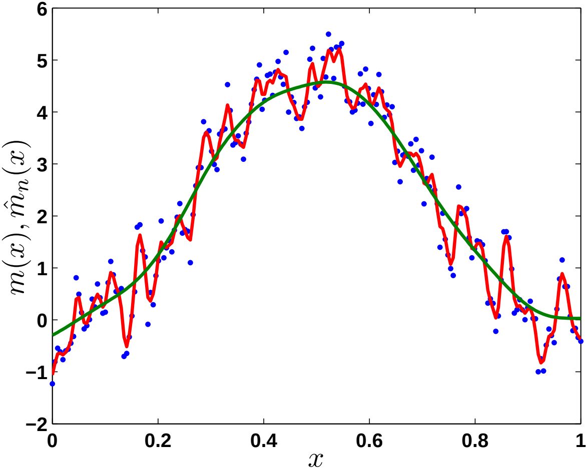

VIOLATION OF I.I.D. ASSUMPTION

What went wrong?

- $Y_i = m(x_i) + e_i$: model selection $\Longrightarrow \text{Cov}[e_i, e_j] = 0$
- In previous example $\text{Cov}[e_i, e_j] \neq 0$
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Suppose there are two technology stocks. If they are affected by the same industry trends, their prices will tend to rise or fall together.

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Housing prices. Sensitive to offer and demand.

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Housing prices. Sensitive to offer and demand.

Example 3

In our toy example: e_{i+1} was affected by the value of e_i and so on...

Removing correlation effects: main theorem

Breakdown bandwidth selection procedures, smoother stays consistent!!

Theorem

Assume $x \equiv i/n$, $x \in [0,1]$, $\mathbf{E}[e] = 0$, $\text{Cov}[e_i, e_{i+k}] = \mathbf{E}[e_i e_{i+k}] = \gamma_k$ *and* $\gamma_k \sim k^{-a}$ *for some* $a > 2$. *Assume that* $Y_i = m(x_i) + e_i$ *and*

(C1) K *is Lipschitz continuous at* $x = 0$;

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Further, assume that boundary effects are ignored and that $h \to 0$ *as* $n \to \infty$ *such that* $nh^2 \to \infty$, *then for the NW smoother it follows that*

$$\mathbf{E}[\text{CV}(h)] = \frac{1}{n}\mathbf{E}\sum_{i=1}^{n}\left[m(x_i) - \hat{m}_n^{(-i)}(x_i)\right]^2 + \sigma^2 - \frac{4K(0)}{nh - K(0)}\sum_{k=1}^{\infty}\gamma_k + o(n^{-1}h^{-1})$$

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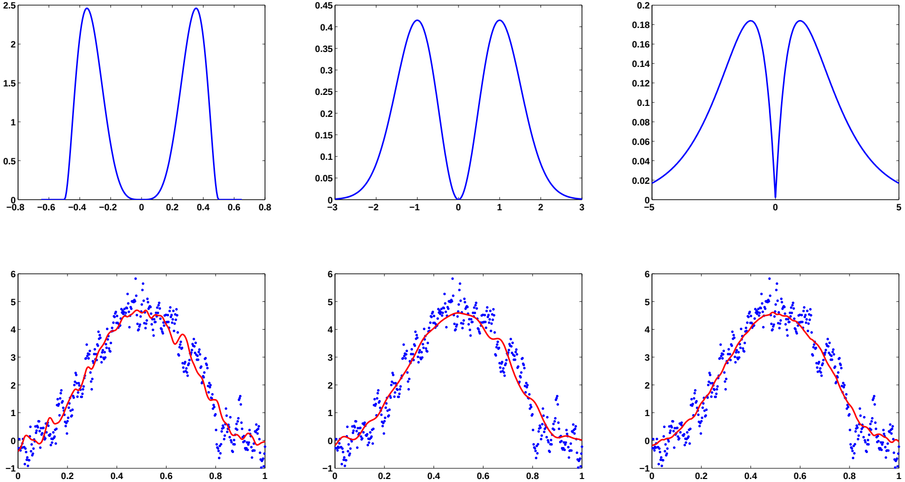
No prior knowledge about correlation structure needed !!

Suitable kernels & drawback



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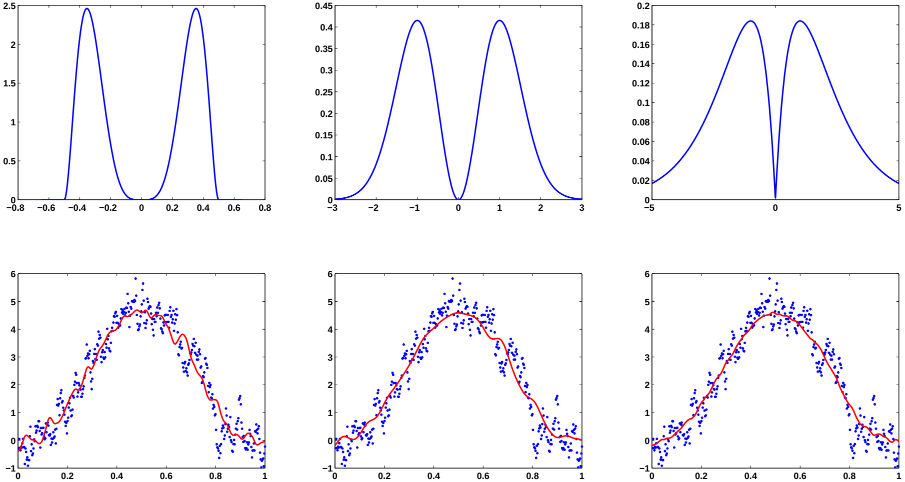
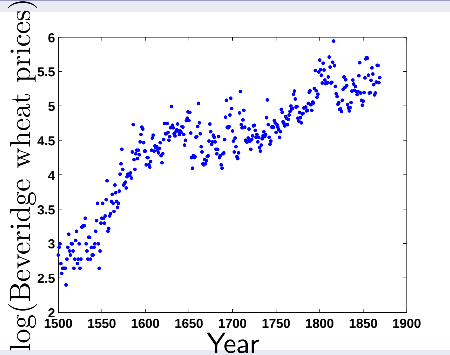


⇒⇒ Decreased Mean Squared Error ⇒⇒

Some real life examples

Beveridge index of wheat prices



U.S. monthly birth rate

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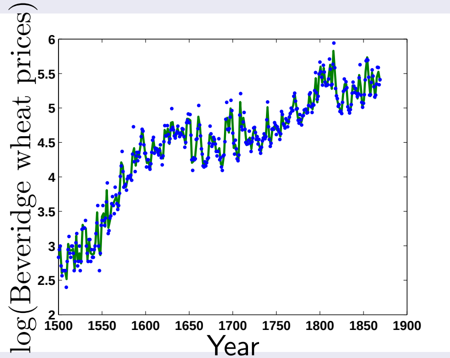

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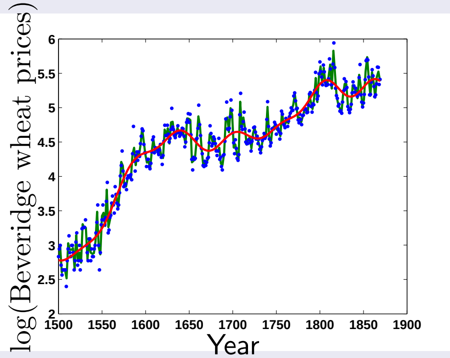

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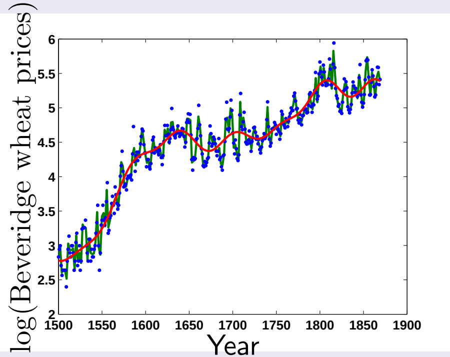

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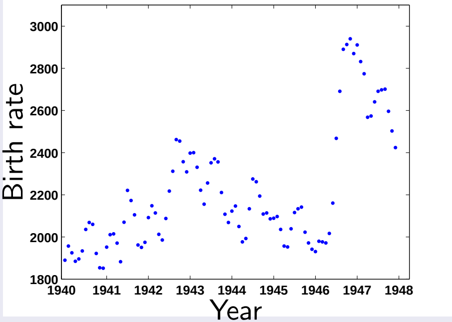

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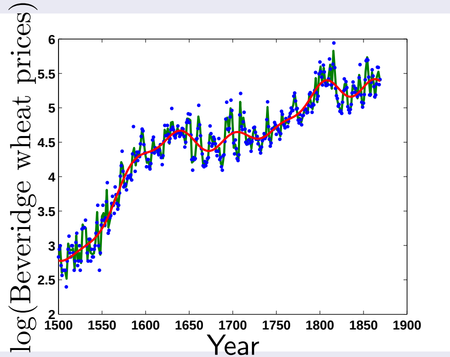

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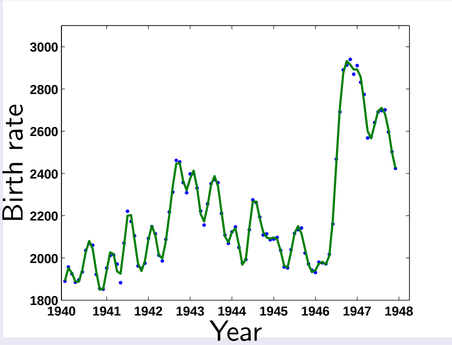

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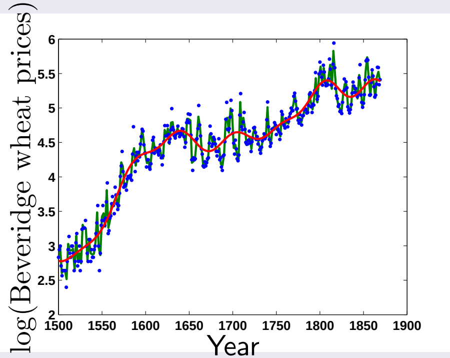

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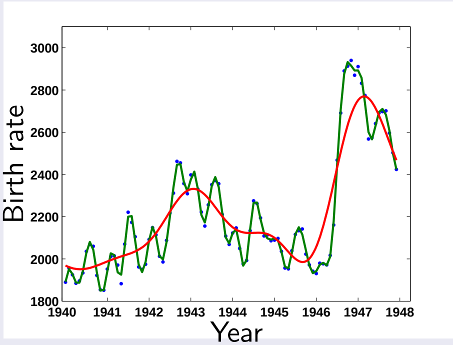

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What are confidence intervals?

- How accurate are our nonparametric estimates?
- Can we say something about the true function m given $\hat{m}_n$?
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  $L_n(x) \leq m(x) \leq U_n(x) \quad \forall x$ for some confidence level α
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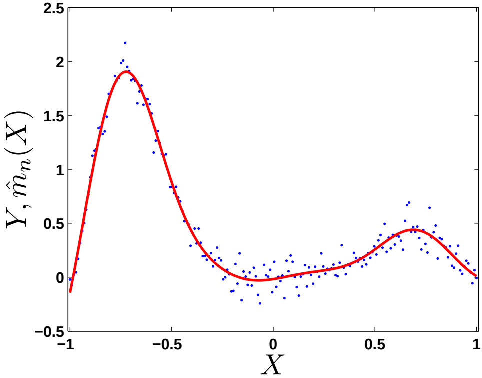

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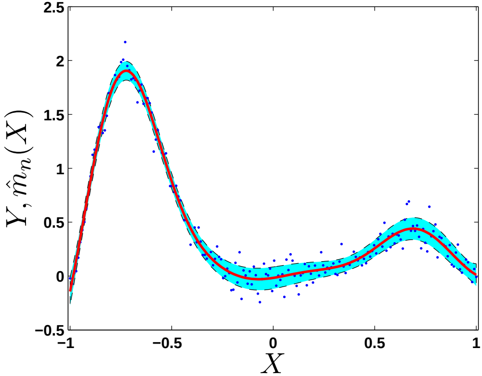

In practice...

In general

These intervals give the user the ability to see how well a certain model explains the true underlying process while taking statistical properties of the estimator into account.

Fault detection

In fault detection: CI are used for reducing the number of false alarms

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Goal of the Thesis

Study the properties of LS-SVM for regression with an emphasis on statistical aspects and develop a framework for large scale data

Main Achievements

- Framework for large data sets
- Method for minimizing model selection criteria score functions
- Robustification of kernel based method
- Weight function with attractive properties
- Framework for correlated errors based on bimodal kernels
- Asymptotic normality of linear smoothers
- Bias & variance estimators for LS-SVM
- Pointwise & simultaneous CI + comparison bootstrap

LS-SVMLab software

- Free available (for research purposes) Matlab toolbox
- `http://www.esat.kuleuven.ac.be/sista/lssvmlab/`
- User's guide with applications (p. 113, De Brabanter *et al*, 2010)

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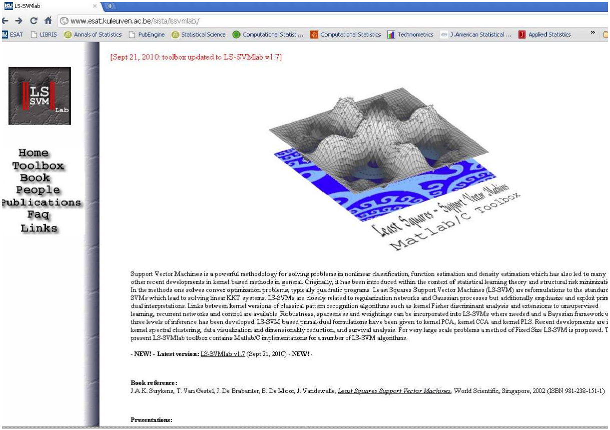

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