Large scale methods

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Lecture 8

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- SVM large scale methods
- Nyström method (GP)
- Fixed size LS-SVM
- Random Fourier features
- Committee networks
- Multilayer approaches

SVM: large scale methods

- Chunking and decomposition methods
- Sequential minimal optimization (SMO)
- Distributed optimization
- Coordinate descent method
- Frank-Wolfe method
- On-line learning, stochastic learning
- Ensemble methods

SMO

- Sequential minimal optimization (SMO) [Platt, 1998]

- Consider dual problem of SVM:

$$\begin{array}{ll} \max\limits_{\alpha} & \sum\limits_i \alpha_i - \frac{1}{2} \sum\limits_{i,j} y_i y_j K(x_i, x_j) \alpha_i \alpha_j \\ \text{subject to} & 0 \leq \alpha_i \leq C, \forall i \\ & \sum_i y_i \alpha_i = 0 \end{array}$$

SMO method:
Consider subproblems of very small size (size 2);
This QP problem can be solved analytically;
Find a Lagrange multiplier α_1 that violates the KKT conditions
Pick a second α_2 and optimize the pair (α_1, α_2)
Repeat the procedure until convergence

Pegasos (1)

- Pegasos (Primal estimated subgradient solver for SVM) [Shalev-Shwartz et al., ICML 2007]:

  Objective function for SVM with hinge loss

$$\frac{\lambda}{2} w^T w + \frac{1}{m} \sum_{(x,y) \in \mathcal{A}_t} L(w,(x,y))$$

  hinge loss $L(w,(x,y)) = \max\{0, 1 - y \langle w, x \rangle\}$
  $\mathcal{A}_t$ random subsample at iteration t
  decision function $\hat{y} = \mathrm{sign}[\langle w, x \rangle]$

Pegasos (2)

Algorithm 1: Pegasos with hinge loss

Data: $\mathcal{S}, \lambda, T, k, \epsilon$

Select w_1 randomly s.t. $\|w^{(1)}\| \leq 1/\sqrt{\lambda}$

for $t = 1 \to T$ **do**

- Set $\eta_t = \frac{1}{\lambda t}$
- Select $\mathcal{A}_t \subseteq \mathcal{S}$, where $|\mathcal{A}_t| = k$
- $\rho = \frac{1}{|\mathcal{S}|} \sum_{(x,y) \in \mathcal{A}_t} (y - \langle w_t, x \rangle), \forall i$
- $\mathcal{A}_t^+ = \{(x, y) \in \mathcal{A}_t : y(\langle w_t, x \rangle + \rho) < 1\}, \forall i$
- $w_{t+\frac{1}{2}} = w_t - \eta_t(\lambda w_t - \frac{1}{k} \sum_{(x,y) \in \mathcal{A}_t^+} yx)$
- $w_{t+1} = \min \left\{ 1, \frac{1/\sqrt{\lambda}}{\|w_{t+\frac{1}{2}}\|} \right\} w_{t+\frac{1}{2}}$
- **if** $\|w_{t+1} - w_t\| \leq \epsilon$ **then**
  - **return** $(w_{t+1}, \frac{1}{|\mathcal{S}|} \sum_{(x,y) \in \mathcal{S}} (y - \langle w_t, x \rangle))$
- **end**

end

return $(w_{T+1}, \frac{1}{|\mathcal{S}|} \sum_{(x,y) \in \mathcal{S}} (y - \langle w_t, x \rangle))$

Nyström method (1)

- Nyström method in Gaussian processes [Williams & Seeger, 2001]

- *"big"* kernel matrix: $\Omega_{(N,N)} \in \mathbb{R}^{N \times N}$
  "small" kernel matrix: $\Omega_{(M,M)} \in \mathbb{R}^{M \times M}$
  (based on random subsample, in practice often $M \ll N$)

- Eigenvalue decomposition of $\Omega_{(M,M)}$:

$$\Omega_{(M,M)} \overline{U} = \overline{U} \, \overline{\Lambda}$$

Nyström method (2)

- Relation to eigenvalues and eigenfunctions of the integral equation

$$\int K(x,x')\phi_i(x)p(x)dx = \lambda_i \phi_i(x')$$

is given by

$$\begin{aligned} \hat{\lambda}_i &= \tfrac{1}{M}\overline{\lambda}_i \\ \hat{\phi}_i(x_k) &= \sqrt{M}\,\overline{u}_{ki} \\ \hat{\phi}_i(x') &= \tfrac{\sqrt{M}}{\overline{\lambda}_i}\sum_{k=1}^{M}\overline{u}_{ki}K(x_k,x') \end{aligned}$$

where $\hat{\lambda}_i$ and $\hat{\phi}_i$ are estimates to λ_i and ϕ_i, respectively, and $\overline{u}_{ki}$ denotes the ki-th entry of the matrix $\overline{U}$.

Nyström method (3)

- For the big matrix:

$$\Omega_{(N,N)}\,\tilde{U} = \tilde{U}\,\tilde{\Lambda}$$

Furthermore, one has

$$\begin{aligned}\tilde{\lambda}_i &= \tfrac{N}{M}\overline{\lambda}_i \\ \tilde{u}_i &= \sqrt{\tfrac{N}{M}}\tfrac{1}{\overline{\lambda}_i}\Omega_{(N,M)}\overline{u}_i\end{aligned}$$

One can show then that

$$\Omega_{(N,N)} \simeq \Omega_{(N,M)}\Omega^{-1}_{(M,M)}\Omega_{(M,N)}$$

where $\Omega_{(N,M)}$ is the $N \times M$ block matrix taken from $\Omega_{(N,N)}$.

Nyström method (4)

- The approximate solution to the big linear system

$$(\Omega_{(N,N)} + I/\gamma)\alpha = y$$

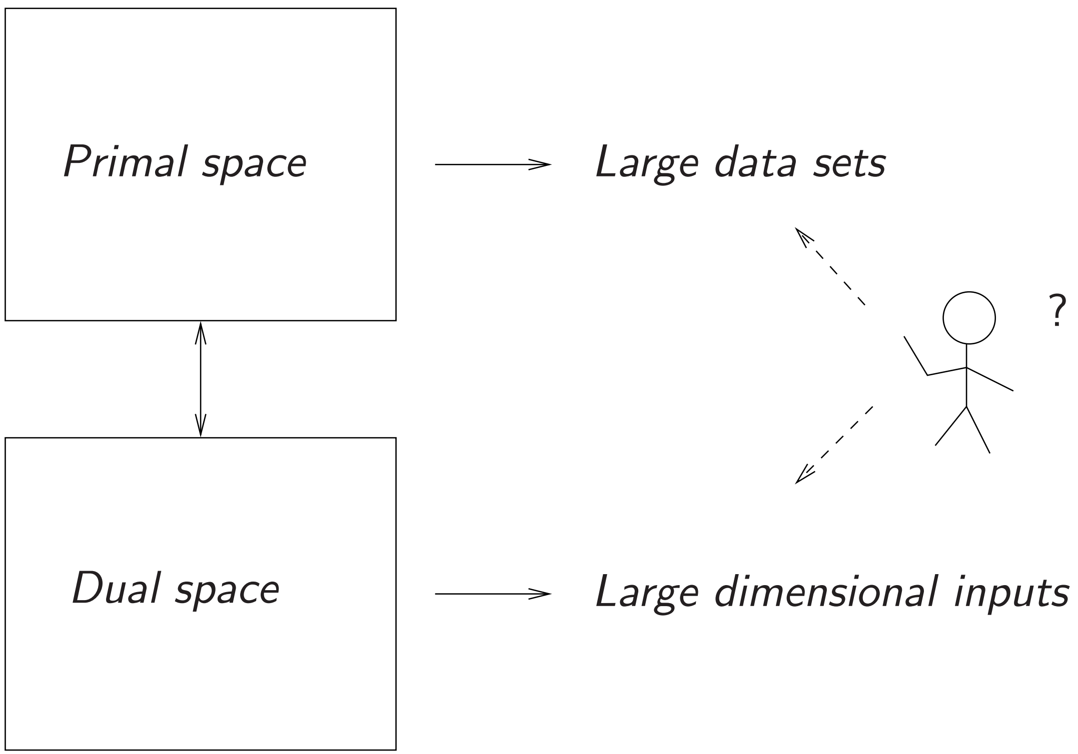
can be written as

$$\alpha = \gamma \left(y - \tilde{U}(\frac{1}{\gamma}I + \tilde{\Lambda}\tilde{U}^T\tilde{U})^{-1}\tilde{\Lambda}\tilde{U}^T y \right)$$

by applying Sherman-Morrison-Woodbury formula

- Some numerical difficulties pointed out by Fine & Scheinberg (2001).

Computation in primal or dual space?



Fixed Size LS-SVM (1)

- Model in primal space:

$$\min_{w\in\mathbb{R}^{n_h},b\in\mathbb{R}} \frac{1}{2}w^T w + \gamma\,\frac{1}{2}\sum_{k=1}^{N}\left(y_k - (w^T\varphi(x_k)+b)\right)^2.$$

For a linear model one can solve the primal problem (one knows the feature map: $\varphi(x_k) = x_k$)

- Can we do this for the nonlinear case too?

- Employ the Nyström method to get an approximation to the feature map

$$\tilde{\varphi}_i(x') = \sqrt{\tilde{\lambda}_i}\,\hat{\phi}_i(x') = \frac{\sqrt{M}}{\sqrt{\tilde{\lambda}_i}}\sum_{k=1}^{M}\overline{u}_{ki}K(x_k,x')$$

assuming a fixed size M.

Fixed Size LS-SVM (2)

- The model becomes then

$$\begin{aligned} y(x) &= w^T \tilde{\varphi}(x) + b \\ &= \sum_{i=1}^{M} w_i \frac{\sqrt{M}}{\sqrt{\lambda_i}} \sum_{k=1}^{M} \overline{u}_{ki} K(x_k, x) + b. \end{aligned}$$

  The support values corresponding to the number of M support vectors equal

$$\alpha_k = \sum_{i=1}^{M} w_i \frac{\sqrt{M}}{\sqrt{\lambda_i}} \overline{u}_{ki}$$

  when ones represent the model as $y(x) = \sum_{k=1}^{M} \alpha_k K(x_k, x) + b$.

- How to select a working set of M support vectors?

Selection of subset

- random
- quadratic Renyi entropy

Fixed Size LS-SVM: Selection of SV

- Link between Nyström method, kernel PCA, density estimation and entropy criteria [Girolami, 2002]. The quadratic Renyi entropy

$$H_R = -\log \int p(x)^2 dx$$

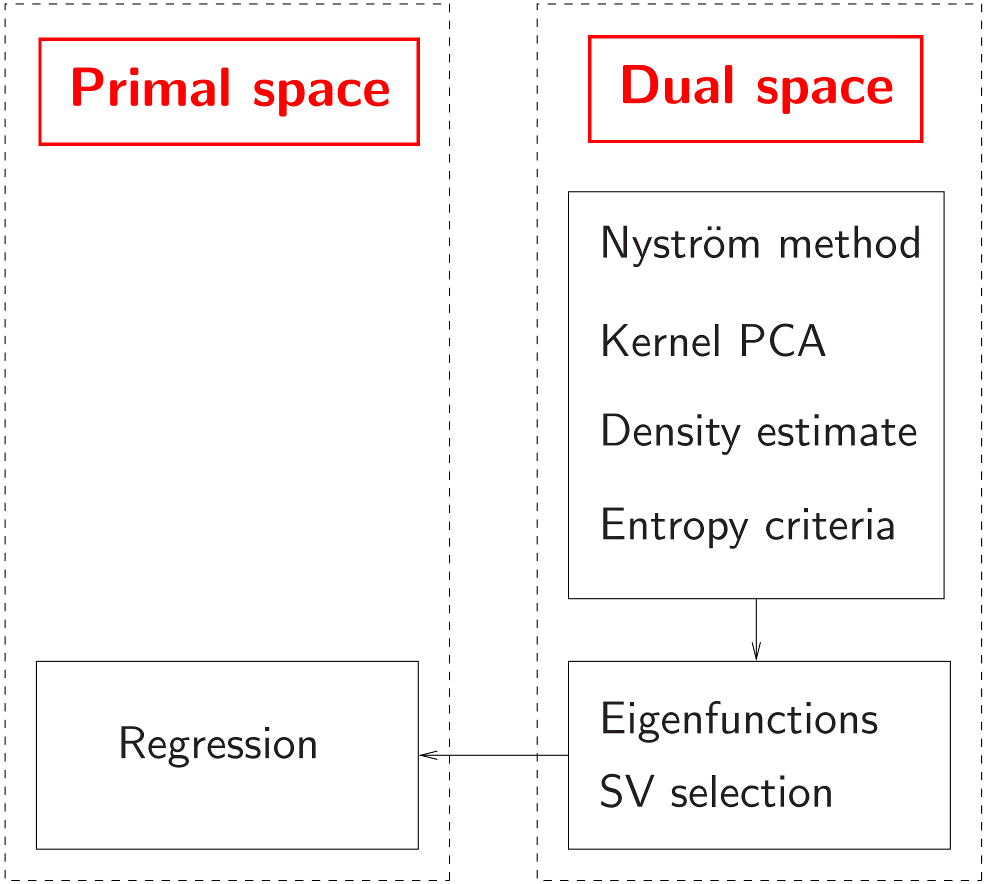
has been related to kernel PCA and density estimation with

$$\int \hat{p}(x)^2 dx = \frac{1}{N^2} 1_v^T \Omega 1_v$$

where $1_v = [1; 1; ...; 1]$ and a normalized kernel is assumed with respect to density estimation.

- Fixed Size LS-SVM: Take a working set of M support vectors and select vectors according to the entropy criterion (instead of a random subsample as in the Nyström method).

Fixed-size kernel method



Modelling in view of primal-dual representations
Link Nyström approximation (GP) - kernel PCA - density estimation

[Suykens et al., 2002]: primal space estimation, sparse, large scale

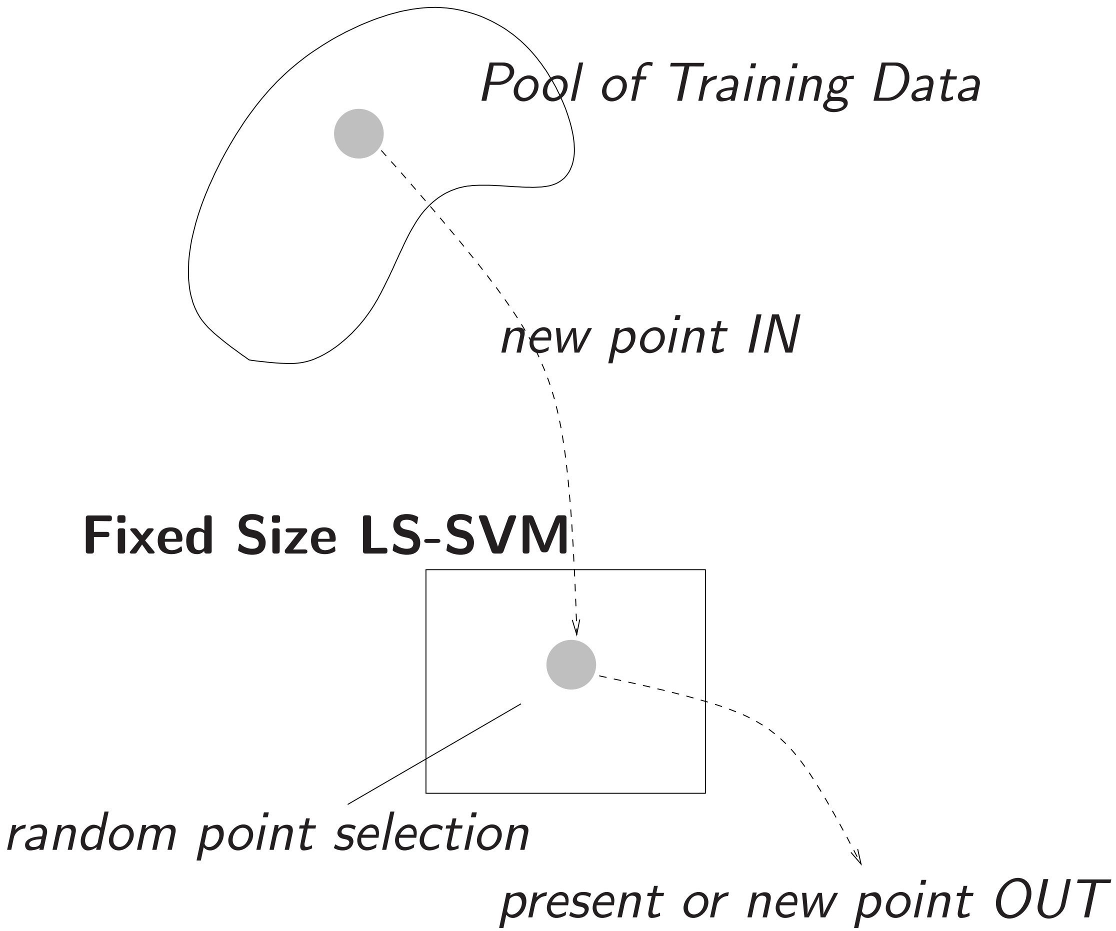
Fixed-size method: using quadratic Renyi entropy (1)

Algorithm:

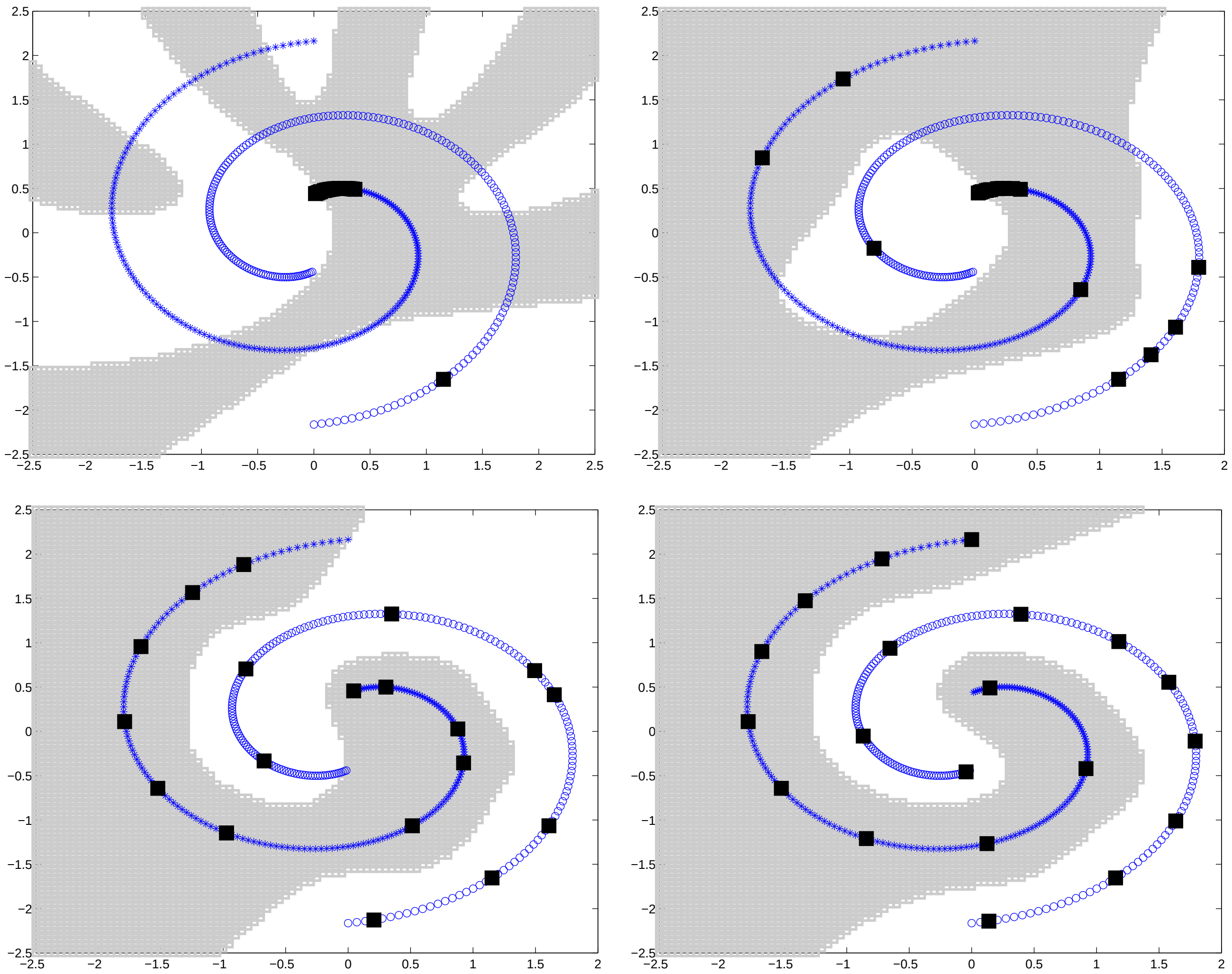
1. Given N training data
2. Choose a working set with fixed size M (i.e. M support vectors) (typically $M \ll N$).
3. Randomly select a SV $\boxed{x^*}$ from the working set of M support vectors.
4. Randomly select a point $\boxed{x^{t*}}$ from the training data and replace x^* by x^{t*}.
   If the entropy increases by taking the point x^{t*} instead of x^* then this point x^{t*} is accepted for the working set of M SVs, otherwise the point x^{t*} is rejected (and returned to the training data pool) and the SV x^* stays in the working set.
5. Calculate the entropy value for the present working set. The quadratic Renyi entropy equals $H_R = -\log \frac{1}{M^2} \sum_{ij} \Omega_{(M,M)_{ij}}$.

[Suykens et al., 2002]

Fixed-size method: using quadratic Renyi entropy (2)

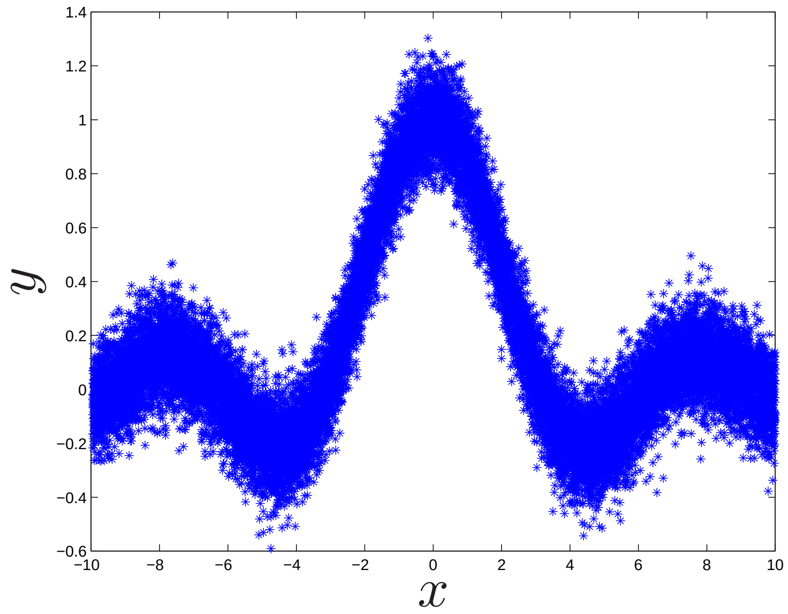


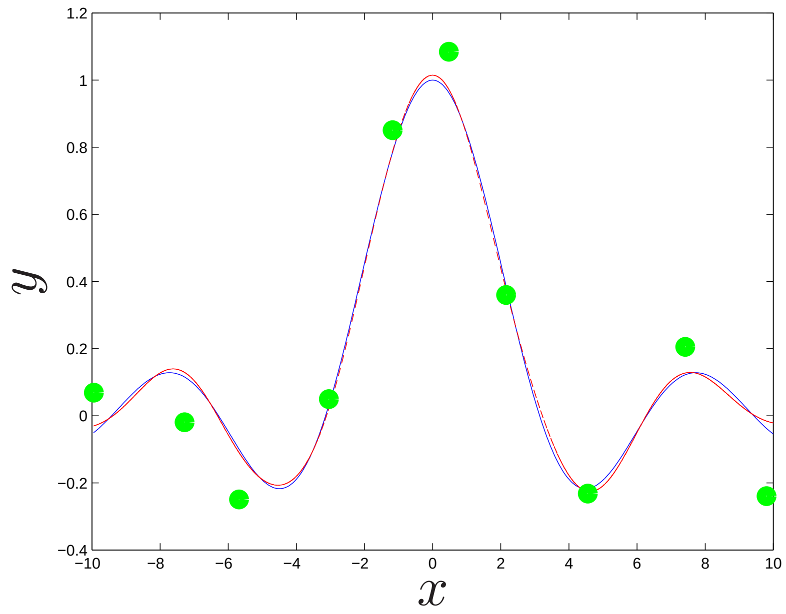
Subset selection using quadratic Renyi entropy: example



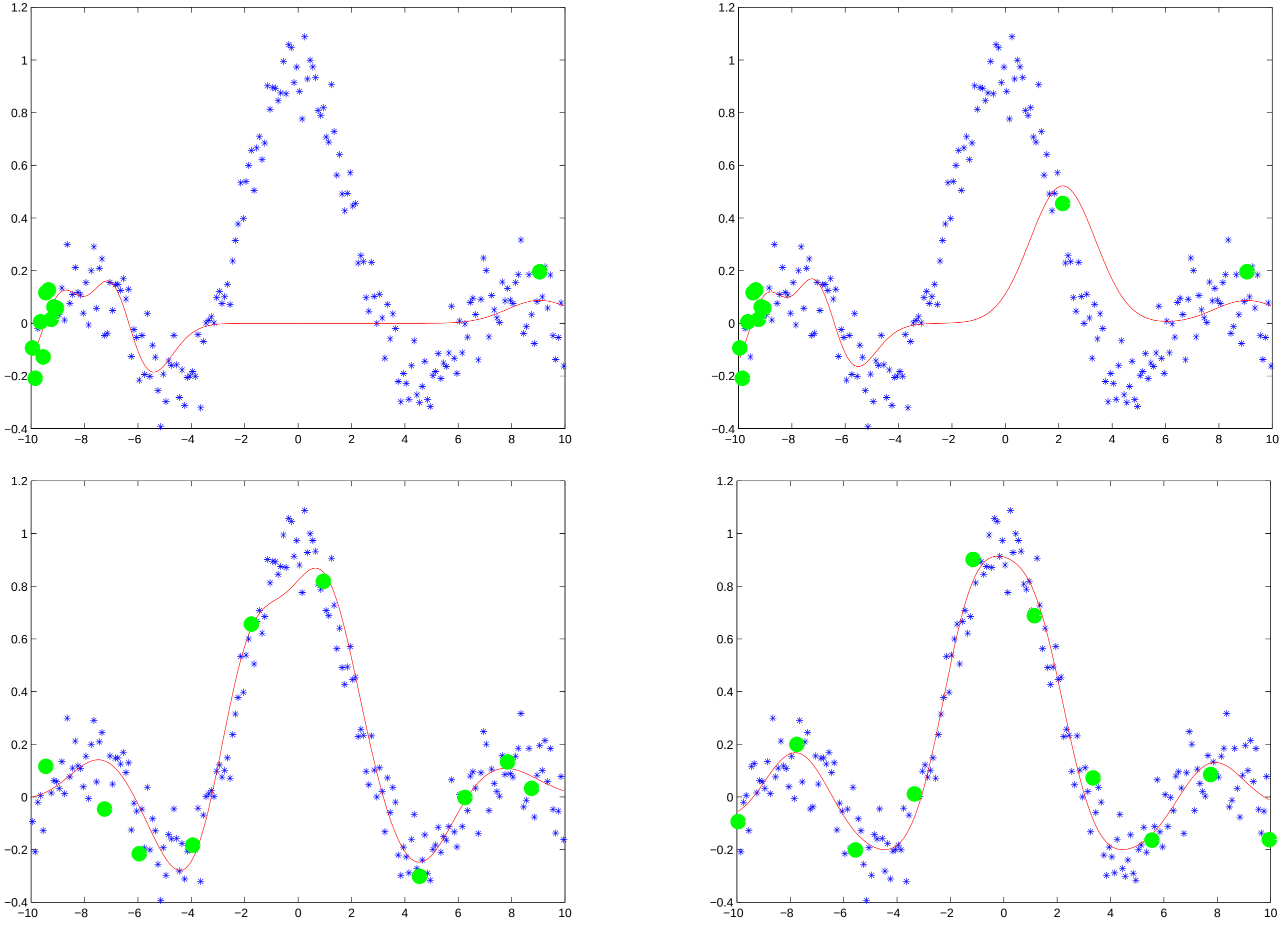
Fixed-size LS-SVM: regression example (1)

Sinc function (20.000 data, 10 SV)

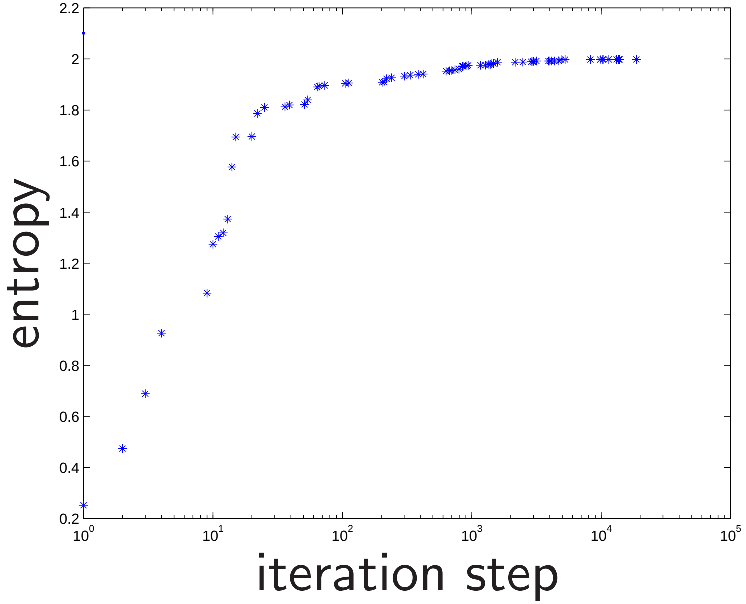


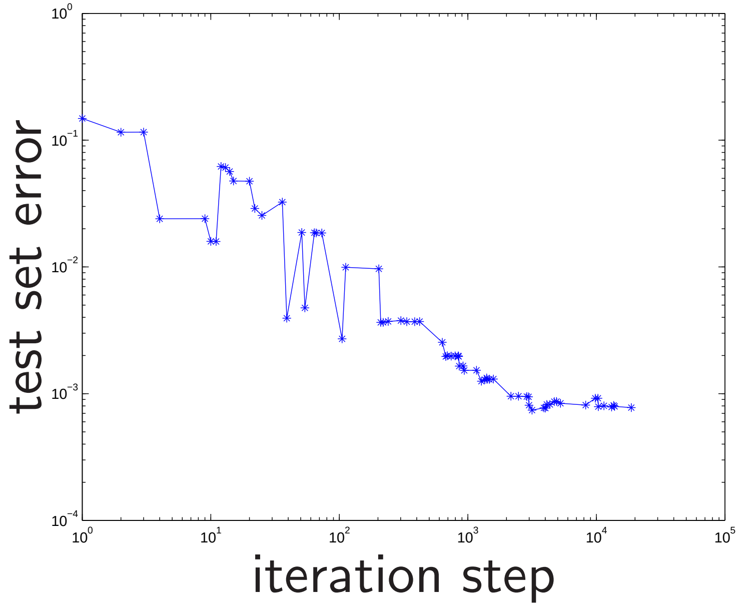


Fixed-size LS-SVM: regression example (2)

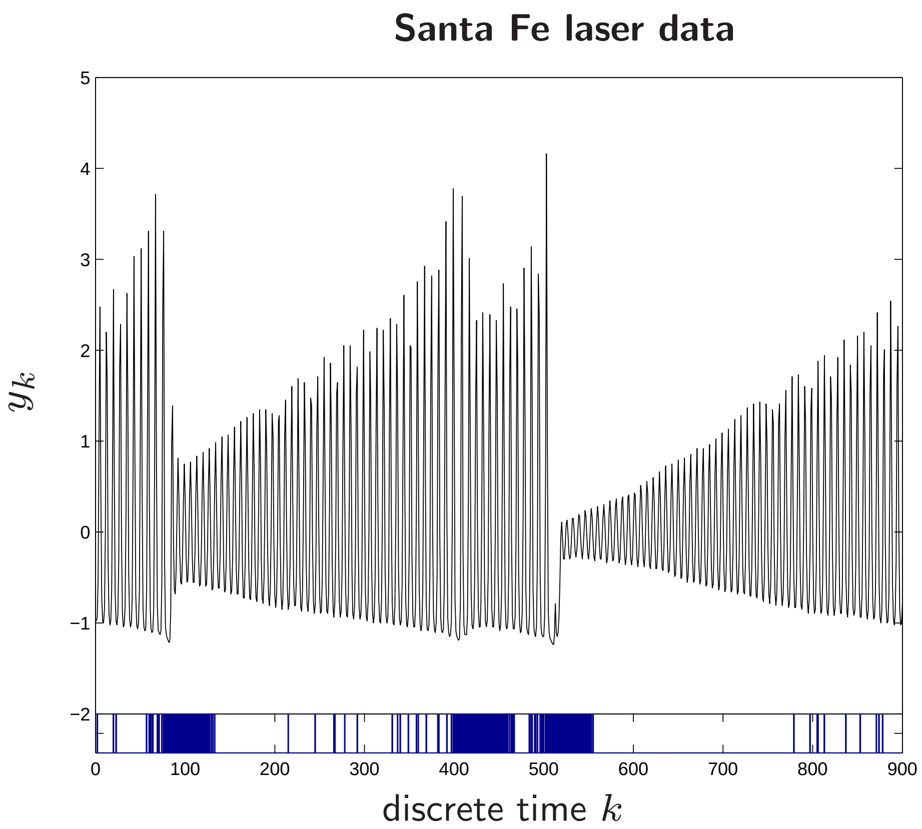


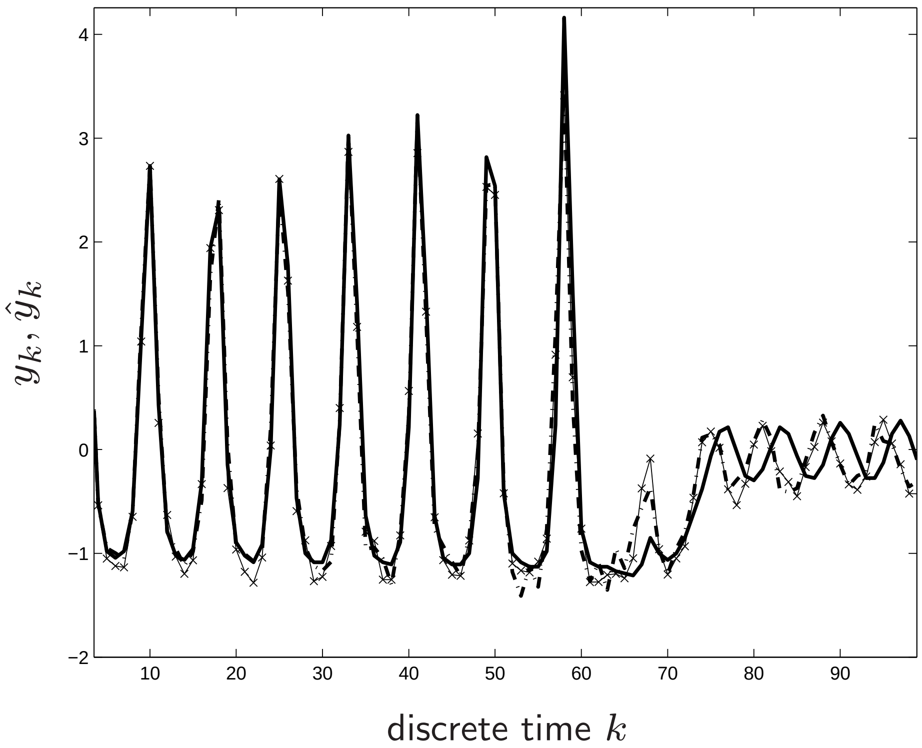
Fixed-size LS-SVM: regression example (3)





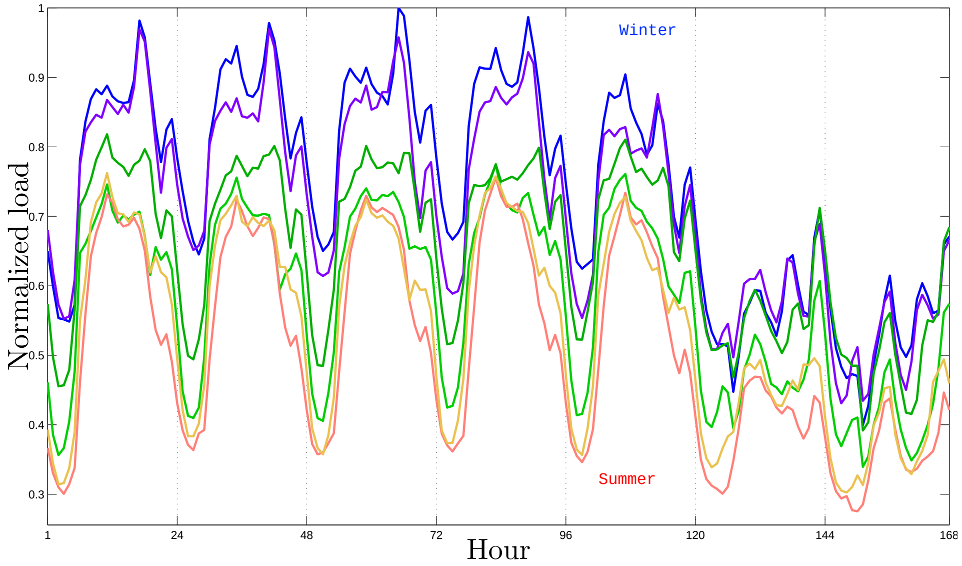
Fixed-size method: example time-series prediction





Training: $\hat{y}_{k+1} = f(y_k, y_{k-1}, ..., y_{k-p})$
Iterative prediction: $\hat{y}_{k+1} = f(\hat{y}_k, \hat{y}_{k-1}, ..., \hat{y}_{k-p})$
[Espinoza et al., 2003]

Electricity load forecasting



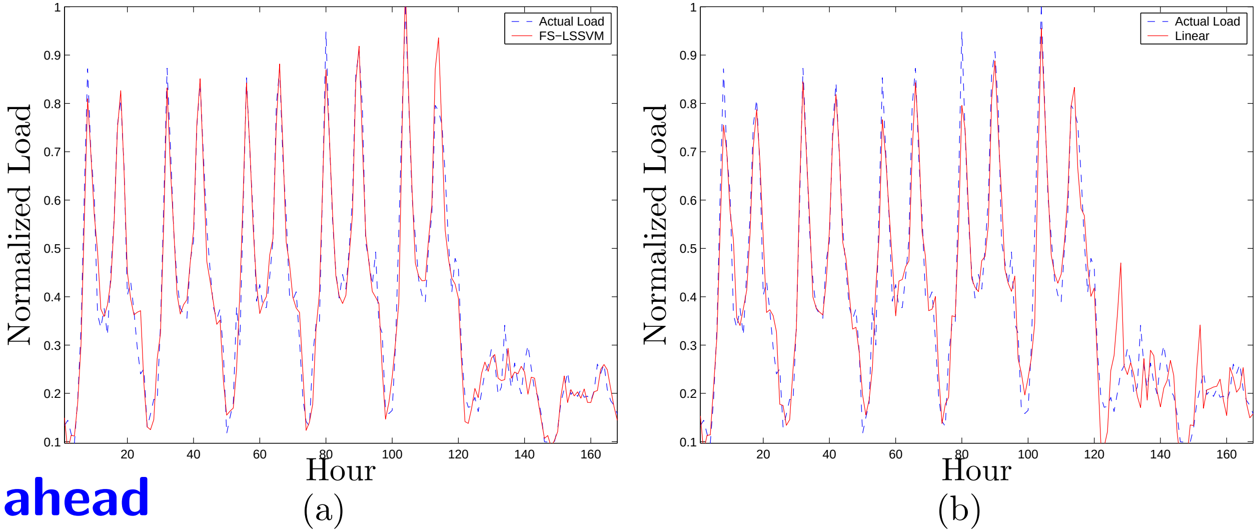
Short-term load forecasting, important for power generation decisions
Hourly load from substations in Belgian grid (ELIA transmission operator)
Seasonal/weekly/intra-daily patterns [Espinoza et al., IEEE CSM 2007]

NARX and AR-NARX model structures: 98 explanatory variables:

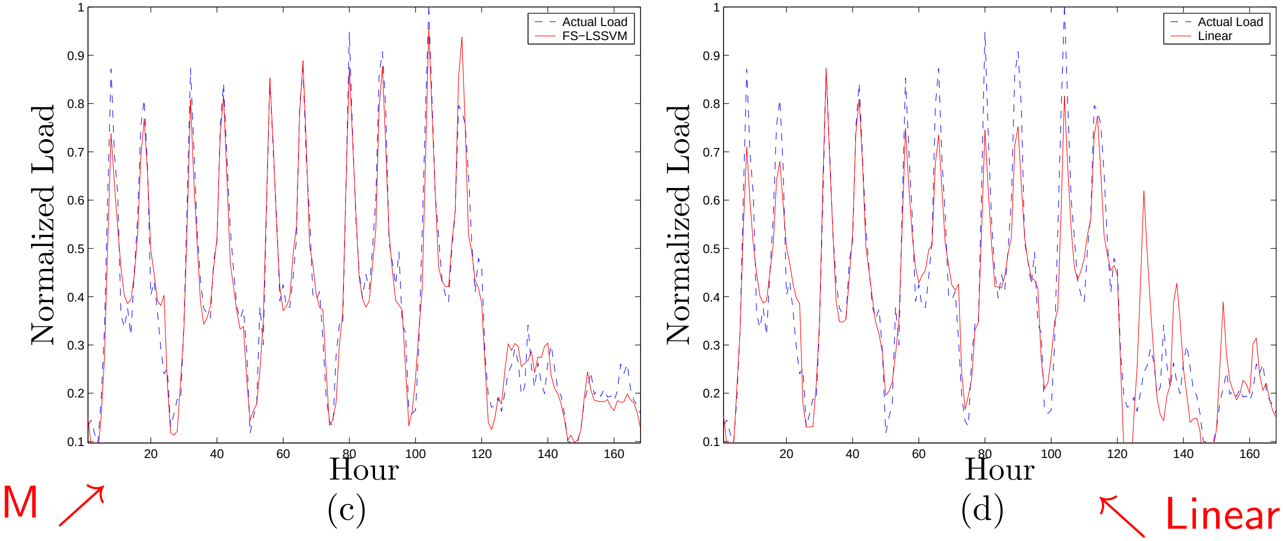
- *lagged load values previous two days (48)*
- *effect of temperature on cooling and heating requirements (3)*
- *calendar information: month, day, hour indications (43)*

Electricity load forecasting (2)

1-hour ahead



24-hours ahead



Fixed-size LS-SVM ↗

↖ Linear ARX model

[Espinoza, Suykens, Belmans, De Moor, IEEE CSM 2007]

Fixed-size method: performance in classification

	pid	spa	mgt	adu	ftc
N	768	4601	19020	45222	581012
N_{cv}	512	3068	13000	33000	531012
N_{test}	256	1533	6020	12222	50000
d	8	57	11	14	54
FS-LSSVM (# SV)	150	200	1000	500	500
C-SVM (# SV)	290	800	7000	11085	185000
ν-SVM (# SV)	331	1525	7252	12205	165205
RBF FS-LSSVM	76.7(3.43)	92.5(0.67)	86.6(0.51)	85.21(0.21)	81.8(0.52)
Lin FS-LSSVM	77.6(0.78)	90.9(0.75)	77.8(0.23)	83.9(0.17)	75.61(0.35)
RBF C-SVM	75.1(3.31)	92.6(0.76)	85.6(1.46)	84.81(0.20)	81.5(no cv)
Lin C-SVM	76.1(1.76)	91.9(0.82)	77.3(0.53)	83.5(0.28)	75.24(no cv)
RBF ν-SVM	75.8(3.34)	88.7(0.73)	84.2(1.42)	83.9(0.23)	81.6(no cv)
Maj. Rule	64.8(1.46)	60.6(0.58)	65.8(0.28)	83.4(0.1)	51.23(0.20)

- Fixed-size (FS) LSSVM: good performance and sparsity wrt C-SVM and ν-SVM
- Challenging to achieve high performance by very sparse models

[De Brabanter et al., CSDA 2010]

Two stages of sparsity

primal	
dual	subset selection Nyström approximation

Two stages of sparsity

	stage 1
primal	FS model estimation
	$\uparrow$
dual	subset selection Nyström approximation

Two stages of sparsity

	stage 1		stage 2
primal	FS model estimation	$\longrightarrow$	reweighted ℓ_1
	$\uparrow$		
dual	subset selection Nyström approximation		

Synergy between parametric & kernel-based models

[Mall & Suykens, IEEE-TNNLS, 2015], reweighted ℓ_1 [Candes et al., 2008]

Random Fourier Features

- Proposed by [Rahimi & Recht, 2007].

- It requires a positive definite shift-invariant kernel $K(x, y) = K(x - y)$. One obtains a randomized feature map $z(x) : \mathbb{R}^d \to \mathbb{R}^{2D}$ so that

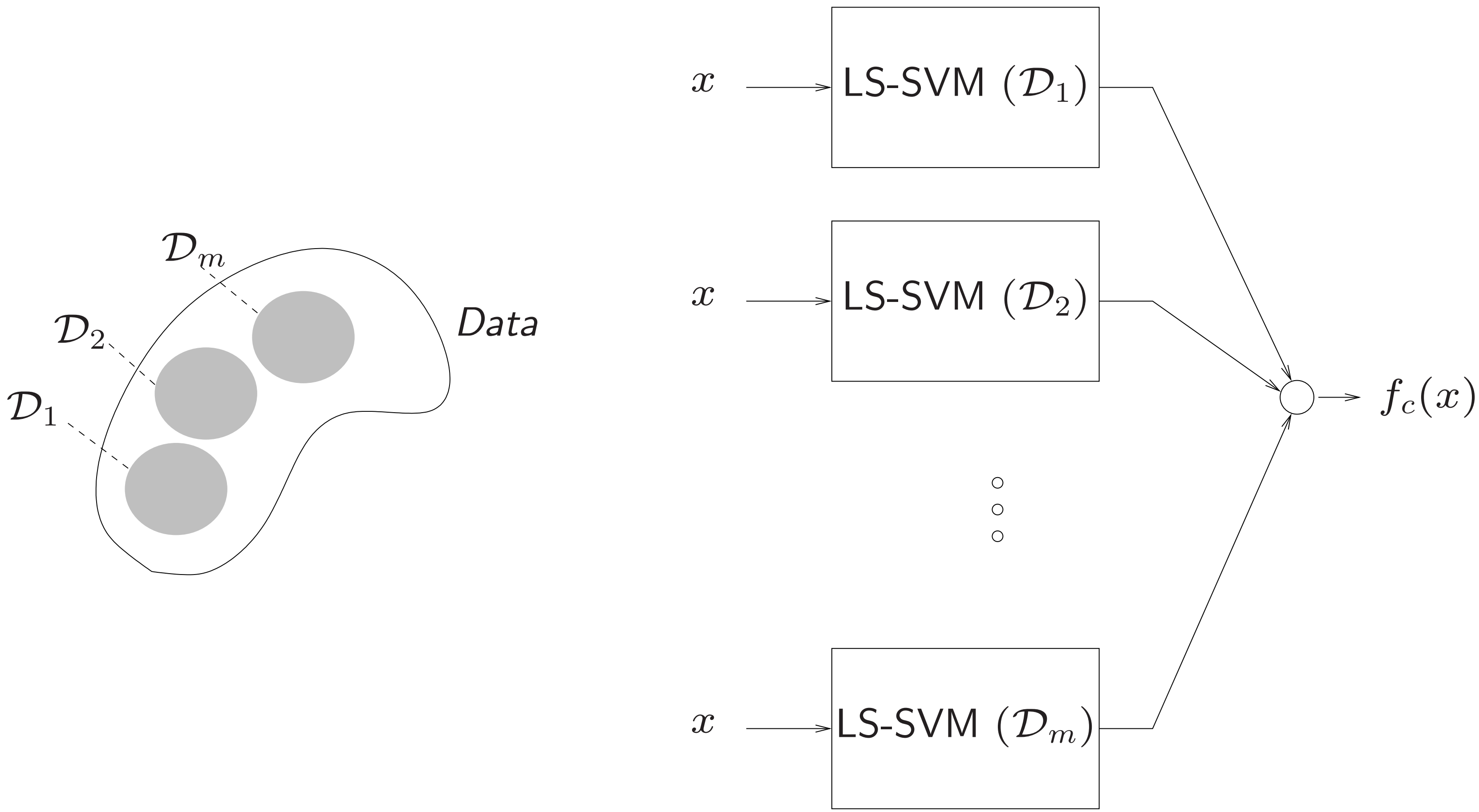
$$z(x)^T z(y) \simeq K(x - y).$$

- Compute the Fourier transform p of the kernel K:

$$p(\omega) = \frac{1}{2\pi} \int \exp(-j\omega^T \Delta) K(\Delta) d\Delta$$

Draw D iid samples $\omega_1, ..., \omega_D \in \mathbb{R}^d$ from p.
Obtain $z(x) = \sqrt{\frac{1}{D}} [\cos(\omega_1^T x) ... \cos(\omega_D^T x) \sin(\omega_1^T x) ... \sin(\omega_D^T x)]^T$.

Committee network of LS-SVMs (1)



Committee network of LS-SVMs (2)

- The committee network that consists of the m submodels takes the form

$$
\begin{aligned}
f_c(x) &= \sum_{i=1}^{m} \beta_i f_i(x) \\
&= h(x) + \sum_{i=1}^{m} \beta_i \epsilon_i(x)
\end{aligned}
$$

where $\sum_{i=1}^{m} \beta_i = 1$, $h(x)$ is the true function to be estimated and $\epsilon_i(x) = f_i(x) - h(x)$ where

$$
f_i(x) = \sum_{k=1}^{N_i} \alpha_k^{(i)} K^{(i)}(x, x_k) + b^{(i)}
$$

is the i-th LS-SVM model trained on the data $\{x_k, y_k\}_{k=1}^{N_i}$ with resulting support values $\alpha_k^{(i)}$, bias term $b^{(i)}$ and kernel $K^{(i)}(\cdot, \cdot)$ for the i-th submodel and $i = 1, ..., m$ with m the number of LS-SVM submodels.

Committee network of LS-SVMs (3)

- One considers the covariance matrix

$$C_{ij} = \mathcal{E}[\epsilon_i(x)\epsilon_j(x)]$$

where in practice one works with a finite-sample approximation

$$C_{ij} = \frac{1}{N}\sum_{k=1}^{N}[f_i(x_k) - y_k][f_j(x_k) - y_k]$$

and the N data are a representative subset of the overall training data set (or the whole training data set itself).

Committee network of LS-SVMs (4)

- The committee error equals

$$
\begin{aligned}
J_c &= \mathcal{E}[\{f_c(x) - h(x)\}^2] = \mathcal{E}[\,(\sum_{i=1}^{m} \beta_i \epsilon_i)\,(\sum_{j=1}^{m} \beta_j \epsilon_j)\,] \\
&\simeq \sum_{i=1}^{m} \sum_{j=1}^{m} \beta_i \beta_j C_{ij} = \beta^T C \beta.
\end{aligned}
$$

An optimal choice of β follows then from

$$
\min_{\beta} \frac{1}{2} \beta^T C \beta \quad \text{such that} \quad \sum_{i=1}^{m} \beta_i = 1.
$$

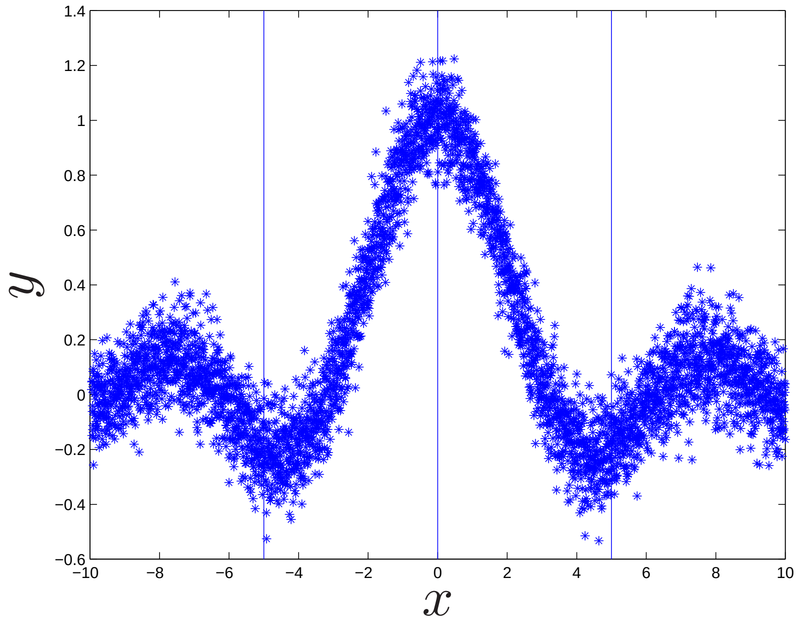
with optimal solution

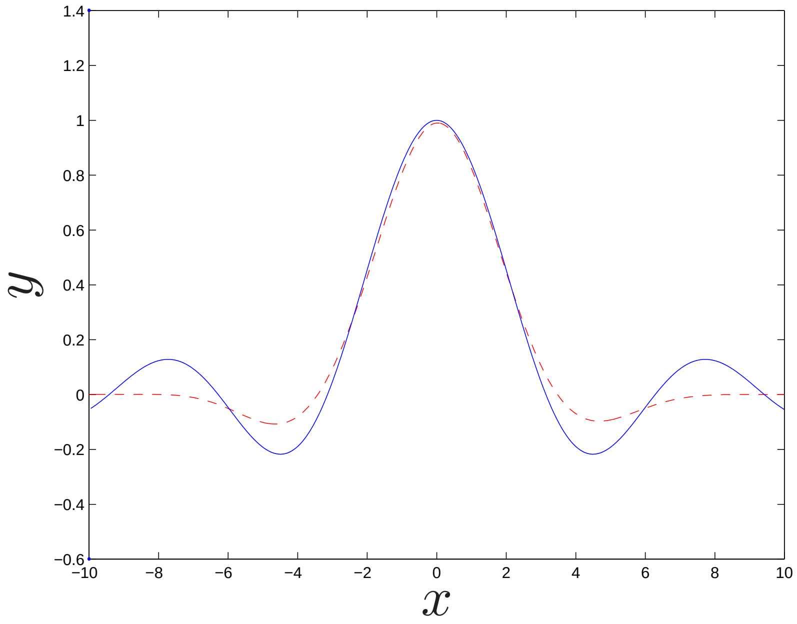
$$
\beta = \frac{C^{-1} 1_v}{1_v^T C^{-1} 1_v}
$$

with $1_v = [1; 1; ...; 1]$.

Example (1)

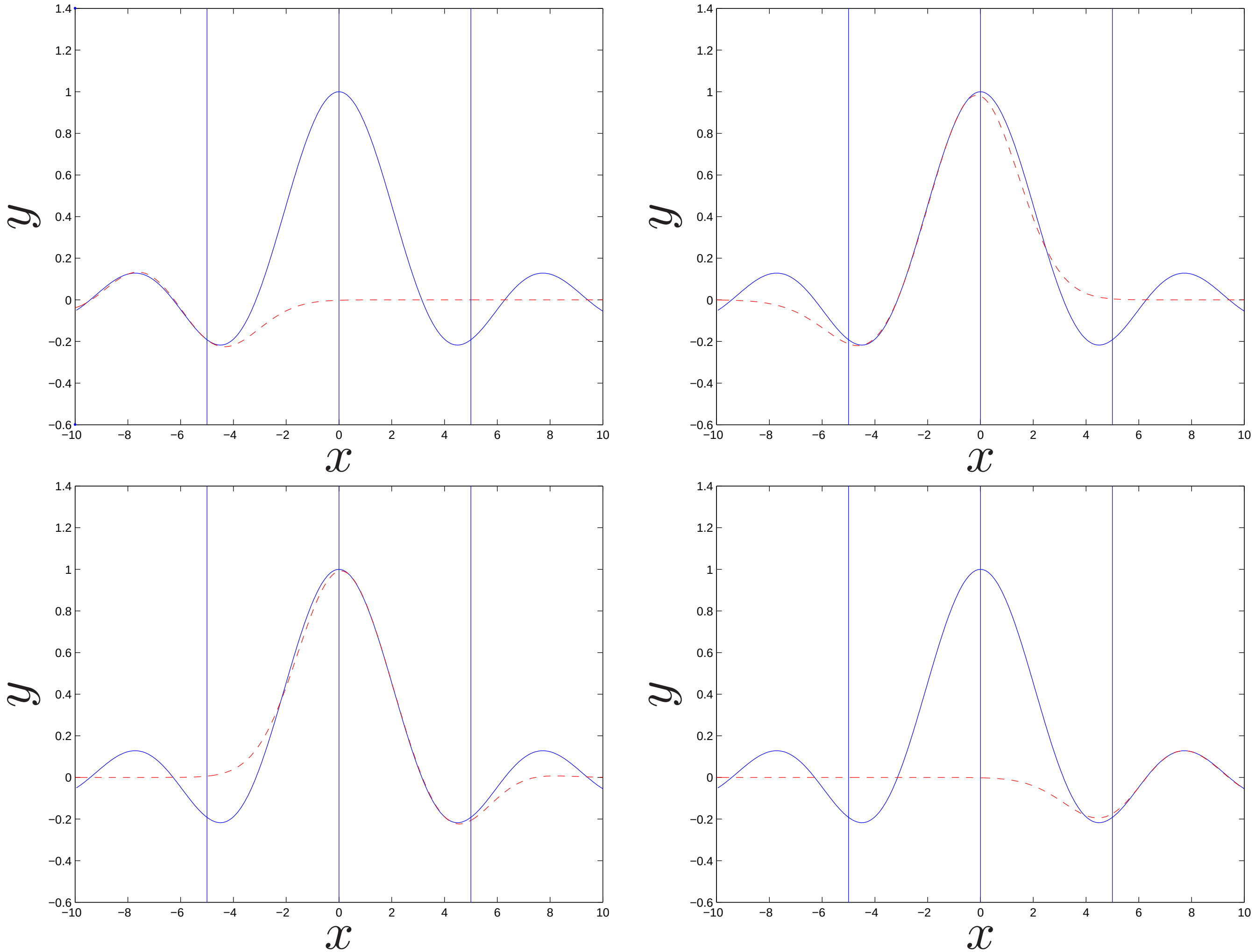
sinc function with 4000 training data



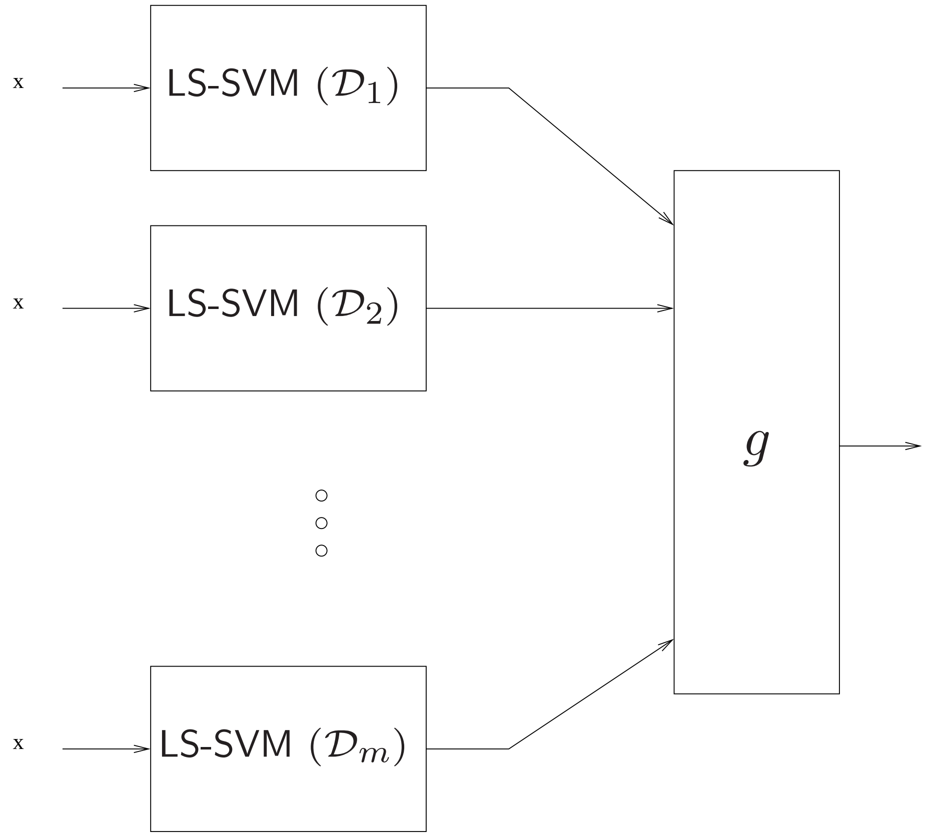


Example (2)

Results of the individual LS-SVM models



Nonlinear combination of LS-SVMs (1)



This results into a multilayer network
(layers of (LS)-SVMs or e.g. MLP + LS-SVM combination)

Nonlinear combination of LS-SVMs (2)

- When taking an MLP in the second layer, the model is described by

$$g(z) = w^T \tanh(Vz + d)$$

with

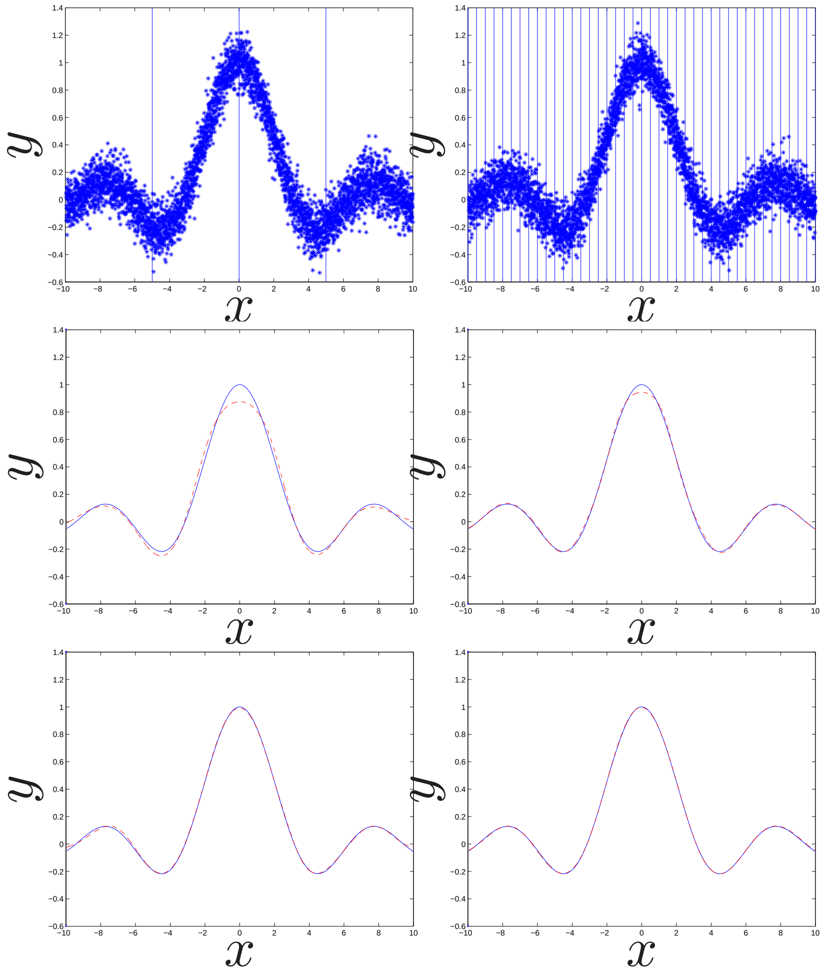
$$z_i(x) = \sum_{k=1}^{N_i} \alpha_k^{(i)} K^{(i)}(x, x_k) + b^{(i)} \ , \ i = 1, ..., m$$

where m denotes the number of individual LS-SVM models whose outputs z_i are the input to a MLP with output weight vector $w \in \mathbb{R}^{n_h}$, hidden layer matrix $V \in \mathbb{R}^{n_h \times m}$ and bias vector $d \in \mathbb{R}^{n_h}$ where n_h denotes the number of hidden units (alternative: linear output layer $g(z) = w^T z + d$).

- The coefficients $\alpha_k^{(i)}, b^{(i)}$ for $i = 1, ..., m$ are the solutions to a number of m linear systems for each of the individual LS-SVMs trained on data sets $\mathcal{D}_i$.

Example (1)

Linear versus nonlinear combinations of trained LS-SVM submodels



Example (2)

Linear versus nonlinear combinations under heavy noise