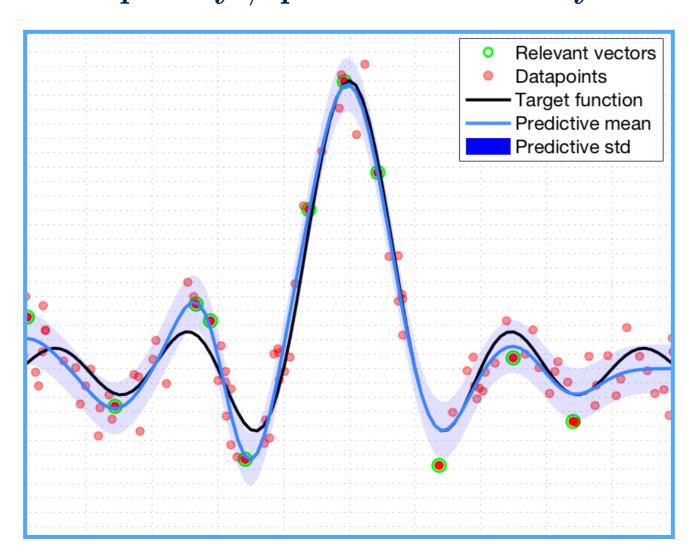
Support Vector Regression vs. Relevance Vector Regression a sparsity / performance study



L.Faury

 ${\bf G. Gallois\text{-}Montbrun} \\ 26/05/2017$ 

H.Hendrikx

## **Outline**

Theoretical reminders on both methods

• Introduction to a sparse-regression metric, experimental justification

Sparse-regression metric based cross-validation

•Performance vs. sparsity discussion

Learn  $f: \mathbb{R}^d \to \mathbb{R}$  thanks to a dataset  $\{X, t\} \in (\mathbb{R}^d)^n \times \mathbb{R}^n$ 

Learn  $f: \mathbb{R}^d \to \mathbb{R}$  thanks to a dataset  $\{X, t\} \in (\mathbb{R}^d)^n \times \mathbb{R}^n$ 

Assuming a Gaussian conditional p.d.f around a linear transformation of features :

$$p(t \mid x, w) = \mathcal{N}(t \mid w^T \phi(x), \beta^{-1})$$

Learn  $f: \mathbb{R}^d \to \mathbb{R}$  thanks to a dataset  $\{X, t\} \in (\mathbb{R}^d)^n \times \mathbb{R}^n$ 

Assuming a Gaussian conditional p.d.f around a linear transformation of features :

$$p(t \mid x, w) = \mathcal{N}(t \mid w^T \phi(x), \beta^{-1})$$

the maximum-likelihood estimator (MLE) writes:

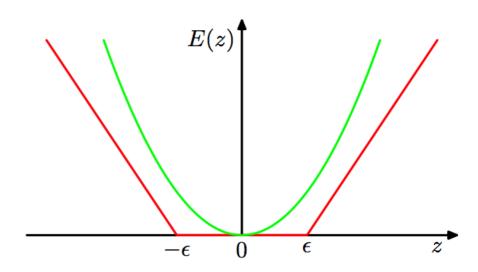
$$\hat{w} = \operatorname{argmax}_{w} p(t \mid X, w)$$

$$= \operatorname{argmin}_{w} \frac{1}{2} \sum_{i=1}^{n} ||w^{t} \phi(x) - t||^{2}$$

<sup>&</sup>lt;sup>1</sup> Vladimir Vapnik, The nature of statistical learning theory, 1995

## Support Vector Regression

• Introduce the  $\varepsilon$ -insensitive<sup>(1)</sup> loss-function.



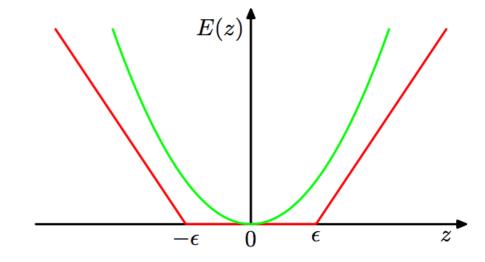
Source: Bishop, Pattern Recognition and Machine Learning (2006)

<sup>&</sup>lt;sup>1</sup> Vladimir Vapnik, The nature of statistical learning theory, 1995

• Introduce the  $\varepsilon$ -insensitive<sup>(1)</sup> loss-function.

$$min_w \frac{C}{n} \sum_n (\xi_n + \hat{\xi}_n) + \frac{1}{2} ||w||^2$$

s.t 
$$\begin{cases} \xi, \hat{\xi} \ge 0 \\ w^T \phi(x_n) + \xi_n + \varepsilon \ge t_n \\ w^T \phi(x_n) - \hat{\xi}_n - \varepsilon \le t_n \end{cases}$$



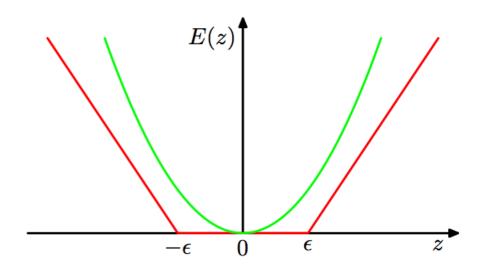
Source: Bishop, Pattern Recognition and Machine Learning (2006)

<sup>&</sup>lt;sup>1</sup> Vladimir Vapnik, The nature of statistical learning theory, 1995

• Introduce the  $\varepsilon$ -insensitive<sup>(1)</sup> loss-function.

$$min_w \frac{C}{n} \sum_n (\xi_n + \hat{\xi}_n) + \frac{1}{2} ||w||^2$$

s.t 
$$\begin{cases} \xi, \hat{\xi} \ge 0 \\ w^T \phi(x_n) + \xi_n + \varepsilon \ge t_n \\ w^T \phi(x_n) - \hat{\xi}_n - \varepsilon \le t_n \end{cases}$$



Source: Bishop, Pattern Recognition and Machine Learning (2006)

• Only points outside the  $\varepsilon$ -tube (active constraints) are used for predictions :

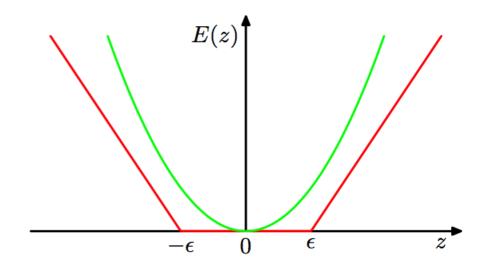
$$y(x) = \sum_{n \in \mathcal{S}} (a_n - \hat{a}_n) k(x, x_n)$$
 Posterior **decision**

<sup>1</sup> Vladimir Vapnik, The nature of statistical learning theory, 1995

• Introduce the  $\varepsilon$ -insensitive<sup>(1)</sup> loss-function.

$$\min_{w} \sum_{n} (\xi_{n} + \hat{\xi}_{n}) + \frac{1}{2} ||w||^{2}$$

s.t 
$$\begin{cases} \xi, \hat{\xi} \ge 0 \\ w^T \phi(x_n) + \xi_n + \varepsilon \ge t_n \\ w^T \phi(x_n) - \hat{\xi}_n - \varepsilon \le t_n \end{cases}$$



Source: Bishop, Pattern Recognition and Machine Learning (2006)

• Only points outside the  $\varepsilon$ -tube (active constraints) are used for predictions :

$$y(x) = \sum_{n \in \mathcal{S}} (a_n - \hat{a}_n) k(x, x_n)$$
 Posterior decision

<sup>1</sup> Vladimir Vapnik, The nature of statistical learning theory, 1995

Relevance Vector Regression<sup>(2)</sup>

<sup>&</sup>lt;sup>2</sup>Tipping Michael, Sparse Bayesian learning and the relevance vector machine, Journal of machine learning research, 2001

## ■Relevance Vector Regression<sup>(2)</sup>

• Provide the predictor with a Gaussian prior :  $w \sim \prod_i \mathcal{N}(w_i \mid 0, \alpha_i^{-1})$ 

$$y(x) = \sum_{n} w_n k(x, x_n)$$

# ■Relevance Vector Regression<sup>(2)</sup>

• Provide the predictor with a Gaussian prior :  $w \sim \prod_i \mathcal{N}(w_i \mid 0, \alpha_i^{-1})$ 

$$y(x) = \sum_{n} w_n k(x, x_n)$$

• Use **type-2 likelihood** (evidence approximation) to determine :

$$(\alpha^*, \beta^*) = \operatorname{argmax}_{\alpha, \beta} \left[ p(t \mid \alpha, \beta) = \int_w p(t \mid w, \beta) p(w \mid \alpha) \right]$$

# ■Relevance Vector Regression<sup>(2)</sup>

• Provide the predictor with a Gaussian prior :  $w \sim \prod_i \mathcal{N}(w_i \mid 0, \alpha_i^{-1})$ 

$$y(x) = \sum_{n} w_n k(x, x_n)$$

• Use **type-2 likelihood** (evidence approximation) to determine :

$$(\alpha^*, \beta^*) = \operatorname{argmax}_{\alpha, \beta} \left[ p(t \mid \alpha, \beta) = \int_w p(t \mid w, \beta) p(w \mid \alpha) \right]$$

• Automatic Relevance Detection : drives some  $\alpha_i$  to  $+\infty$  (sparse model). Others are called **relevant** vectors.

# ■Relevance Vector Regression<sup>(2)</sup>

• Provide the predictor with a Gaussian prior :  $w \sim \prod_i \mathcal{N}(w_i \mid 0, \alpha_i^{-1})$ 

$$y(x) = \sum_{n} w_n k(x, x_n)$$

• Use **type-2 likelihood** (evidence approximation) to determine :

$$(\alpha^*, \beta^*) = \operatorname{argmax}_{\alpha, \beta} \left[ p(t \mid \alpha, \beta) = \int_w p(t \mid w, \beta) p(w \mid \alpha) \right]$$

• Automatic Relevance Detection : drives some  $\alpha_i$  to  $+\infty$  (sparse model). Others are called **relevant** vectors.

• Compute posterior and **predictive distribution** 

# Relevance Vector Regression<sup>(2)</sup>

• Provide the predictor with a Gaussian prior :  $w \sim \prod_i \mathcal{N}(w_i \mid 0, \alpha_i^{-1})$ 

$$y(x) = \sum_{n} w_n k(x, x_n)$$

• Use **type-2 likelihood** (evidence approximation) to determine :

$$(\alpha^*, \beta^*) = \operatorname{argmax}_{\alpha, \beta} \left[ p(t \mid \alpha, \beta) = \int_w p(t \mid w, \beta) p(w \mid \alpha) \right]$$

• Automatic Relevance Detection : drives some  $\alpha_i$  to  $+\infty$  (sparse model). Others are called **relevant** vectors.

• Compute posterior and **predictive distribution** 

Comparison

 $\underline{\text{SVR}}$   $\underline{\text{RVR}}$ 

<sup>&</sup>lt;sup>3</sup>John Platt, Sequential Minimal Optimization: A fast algorithm for training support vector machines. 1998

## Comparison

### <u>SVR</u>

▶ Predictive choice

### RVR

▶ Predictive distribution

<sup>&</sup>lt;sup>3</sup>John Platt, Sequential Minimal Optimization: A fast algorithm for training support vector machines. 1998

### $\underline{SVR}$

- Predictive choice
- ► Held-out method for hyper-parameters (at least 3)

### $\overline{\text{RVR}}$

- ▶ Predictive distribution
- ► Hyper-parameters are determined automatically (except kernel)

<sup>&</sup>lt;sup>3</sup>John Platt, Sequential Minimal Optimization: A fast algorithm for training support vector machines. 1998

### $\underline{SVR}$

- Predictive choice
- Held-out method for hyper-parameters (at least 3)
- ► Mercer kernel

- ▶ Predictive distribution
- ► Hyper-parameters are determined automatically (except kernel)
- ► Arbitrary base functions

<sup>&</sup>lt;sup>3</sup>John Platt, Sequential Minimal Optimization: A fast algorithm for training support vector machines. 1998

### $\underline{SVR}$

- Predictive choice
- ► Held-out method for hyper-parameters (at least 3)
- ► Mercer kernel
- ► **Training** : SMO<sup>(3)</sup> (somewhere between linear and quadratic)

- ▶ Predictive distribution
- ► Hyper-parameters are determined automatically (except kernel)
- ► Arbitrary base functions
- ▶ **Training** : cubic complexity

<sup>&</sup>lt;sup>3</sup>John Platt, Sequential Minimal Optimization: A fast algorithm for training support vector machines. 1998

### $\underline{SVR}$

- Predictive choice
- ► Held-out method for hyper-parameters (at least 3)
- ► Mercer kernel
- ► **Training**: SMO<sup>(3)</sup> (somewhere between linear and quadratic)
- ► **Testing** : linear in the SV

- ▶ Predictive distribution
- ► Hyper-parameters are determined automatically (except kernel)
- ► Arbitrary base functions
- ► **Training** : cubic complexity
- ► **Testing**: linear in the RV

<sup>&</sup>lt;sup>3</sup>John Platt, Sequential Minimal Optimization: A fast algorithm for training support vector machines. 1998

### <u>SVR</u>

- ▶ Predictive choice
- ► Held-out method for hyper-parameters (at least 3)
- ► Mercer kernel
- ▶ **Training** : SMO<sup>(3)</sup> (somewhere between linear and quadratic)
- ► **Testing**: linear in the SV

- ▶ Predictive distribution
- ► Hyper-parameters are determined automatically (except kernel)
- ► Arbitrary base functions
- ▶ **Training** : cubic complexity
- ▶ **Testing** : linear in the RV

<sup>&</sup>lt;sup>3</sup>John Platt, Sequential Minimal Optimization: A fast algorithm for training support vector machines. 1998

Goal

Sparsity / Performance

<sup>&</sup>lt;sup>4</sup>Christopher Bishop, Pattern Recognition Machine Learning, 2006



Sparsity / Performance

• **Question**: Compare the tradeoff found between performance (MSE minimization) and sparsity

<sup>&</sup>lt;sup>4</sup>Christopher Bishop, Pattern Recognition Machine Learning, 2006



## Sparsity / Performance

• **Question**: Compare the tradeoff found between performance (MSE minimization) and sparsity

• Literature<sup>(4)</sup>: RVR reaches sparser models with equivalent generalization skills.

## Sparsity / Performance

• **Question**: Compare the tradeoff found between performance (MSE minimization) and sparsity

• Literature<sup>(4)</sup>: RVR reaches sparser models with equivalent generalization skills.

- <u>Initial idea</u>: Test (**experimentally**) this assertion
  - what is performance?
  - what do we want with sparsity?
  - ▶ how to measure the tradeoff?

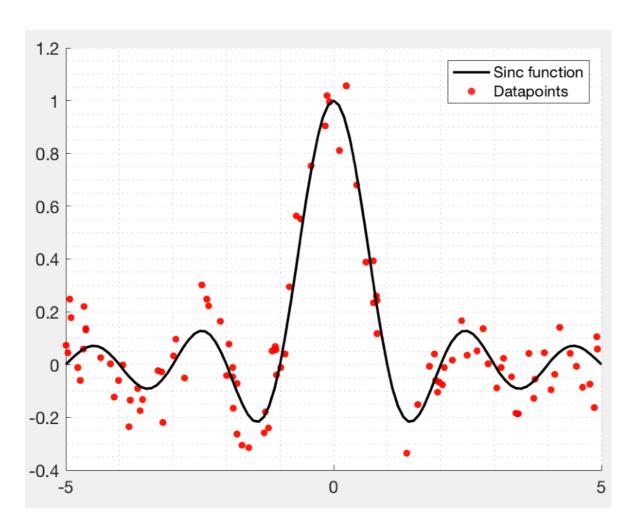
<sup>&</sup>lt;sup>4</sup>Christopher Bishop, Pattern Recognition Machine Learning, 2006

**Datasets** 

<sup>&</sup>lt;sup>5</sup>T.F. Brooks, D.S. Pope, and A.M. Marcolini. Airfoil self-noise and prediction. Technical report NASA. 1989.

#### Datasets





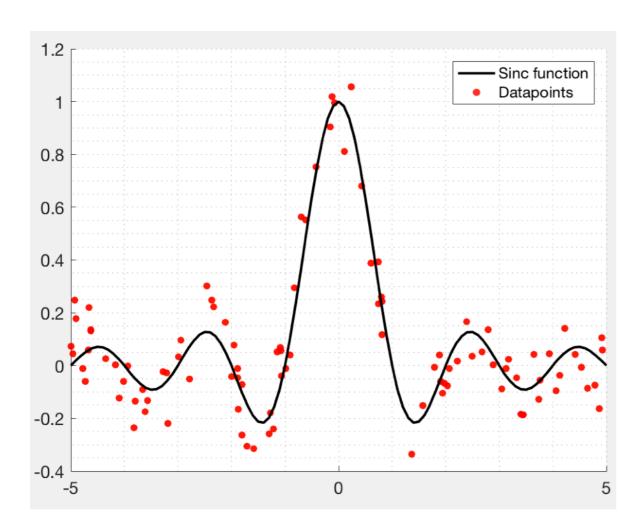
| Dimension | Points | Support | Noise variance | Outlier |
|-----------|--------|---------|----------------|---------|
| 1         | 100    | [-5,5]  | 0.01           | No      |

<sup>5</sup>T.F. Brooks, D.S. Pope, and A.M. Marcolini. Airfoil self-noise and prediction. Technical report NASA. 1989.

## Dataset presentation

#### Datasets





| Dimension | Points | Support | Noise variance | Outlier |
|-----------|--------|---------|----------------|---------|
| 1         | 100    | [-5,5]  | 0.01           | No      |

#### Real (5d)

• Airfoil Self-Noise Data Set (NASA)<sup>(5)</sup>

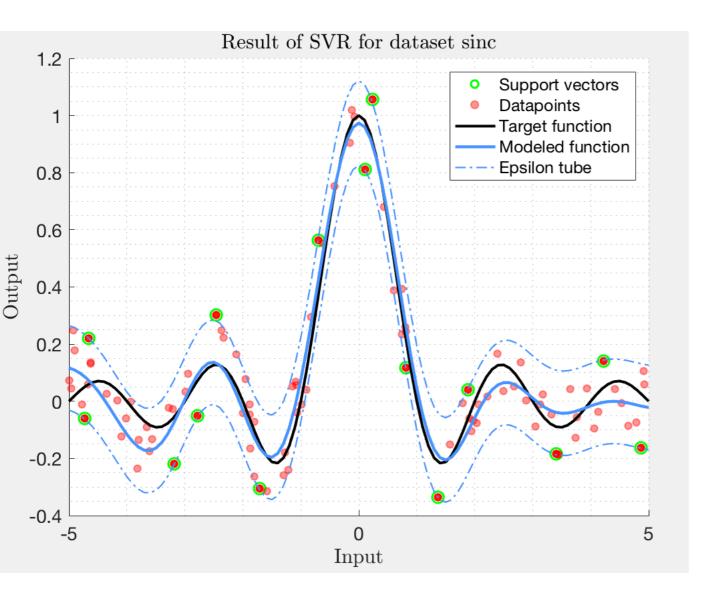
| Dimension | Points |
|-----------|--------|
| 5         | 1503   |

- Predict sound pressure (dB) according to few features :
  - Eigen frequency
  - Angle of attack
  - Chord Length
  - Free stream
  - ▶ Suction side displacement thickness

■ Test Run

### Test Run

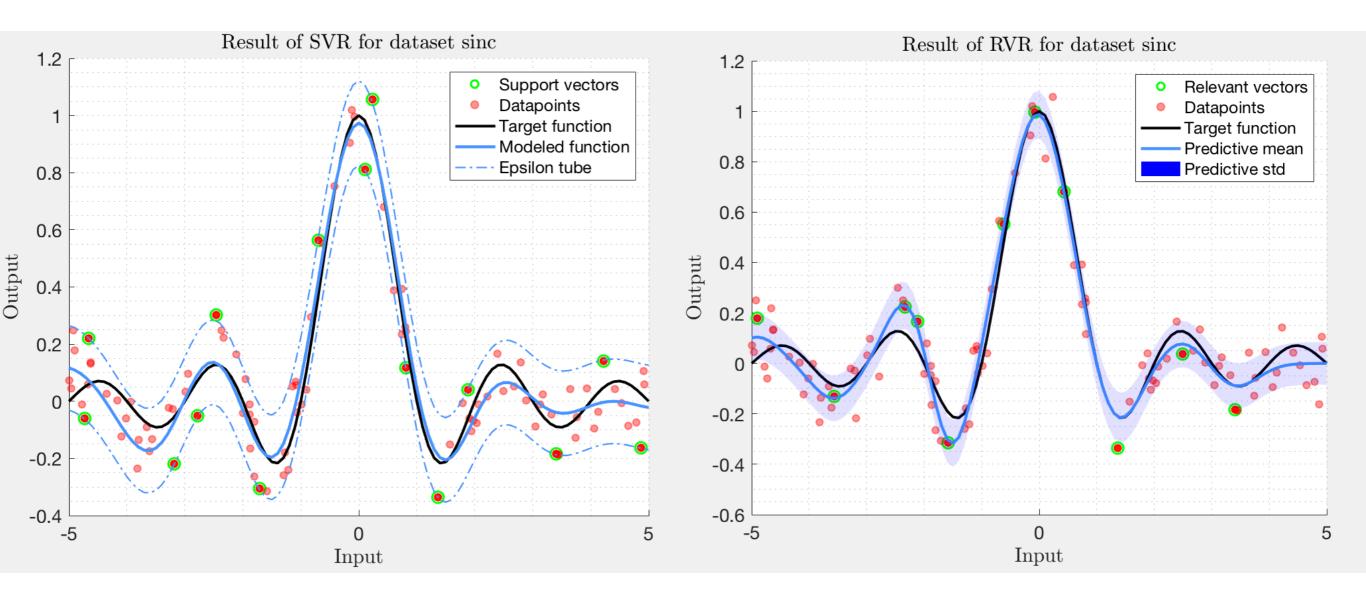
### ■ Test Run



$$\begin{cases} \nu - \text{SVR, RBF kernel with:} \\ \nu = 0.08 \\ C = 8.5 \\ \sigma = 1.4 \text{ (kernel width)} \end{cases}$$

### Test Run

### ■ Test Run



$$\begin{cases} \nu - \text{SVR, RBF kernel with:} \\ \nu = 0.08 \\ C = 8.5 \\ \sigma = 1.4 \text{ (kernel width)} \end{cases}$$

RVR, RBF kernel with:  $\sigma = 1$ 

Intuition

## Sparse Regression Metric

#### Intuition

• Goal: Maximize performance while penalizing complexity

#### Intuition

- Goal: Maximize performance while penalizing complexity
- BIC (Bayesian Information Criterion) for model selection:

$$BIC = -2 \underbrace{\log \mathcal{L}(x)}_{\text{likelihood}} + \underbrace{M \log N}_{\text{model complexity}}$$

#### Intuition

- Goal: Maximize performance while penalizing complexity
- BIC (Bayesian Information Criterion) for model selection:

$$BIC = -2 \underbrace{\log \mathcal{L}(x)}_{\text{likelihood}} + \underbrace{M \log N}_{\text{model complexity}}$$

• Adaptation to regression :

$$-\log \mathcal{L}(x) = \beta N \cdot MSE(x,t)$$
 Gaussian likelihood 
$$M \stackrel{\triangle}{\sim} |SV| = k$$
 complexity = number of support vectors

#### Intuition

- Goal: Maximize performance while penalizing complexity
- BIC (Bayesian Information Criterion) for model selection:

$$BIC = -2 \underbrace{\log \mathcal{L}(x)}_{\text{likelihood}} + \underbrace{M \log N}_{\text{model complexity}}$$

• Adaptation to regression :

$$-\log \mathcal{L}(x) = \beta N \cdot MSE(x,t)$$
 Gaussian likelihood 
$$M \stackrel{\triangle}{\sim} |SV| = k$$
 complexity = number of support vectors

• BICSR (BIC for Sparse Regression)

$$BICSR = \beta N \cdot MSE + k \log N$$

**Experimental Evaluation** 

Experimental Evaluation

• Goal: Evaluate the tradeoff found by the BICSR metric

Experimental Evaluation

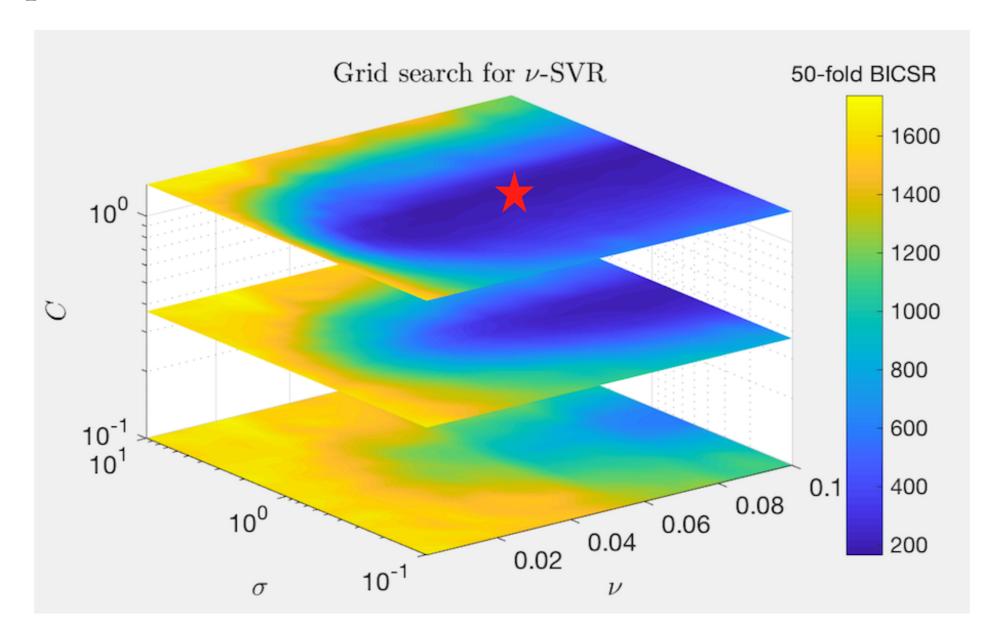
• Goal: Evaluate the tradeoff found by the BICSR metric

- For each method (SVR and RVR):
  - ▶ Cross-validation to find the best hyper-parameters according to BICSR and MSE
  - Compare them with arbitrary models

■ Best hyper-parameters selection

- Best hyper-parameters selection
- Example for SVR with BICSR:

- Best hyper-parameters selection
- Example for SVR with BICSR:



- Best hyper-parameters selection
- Example for SVR with BICSR:

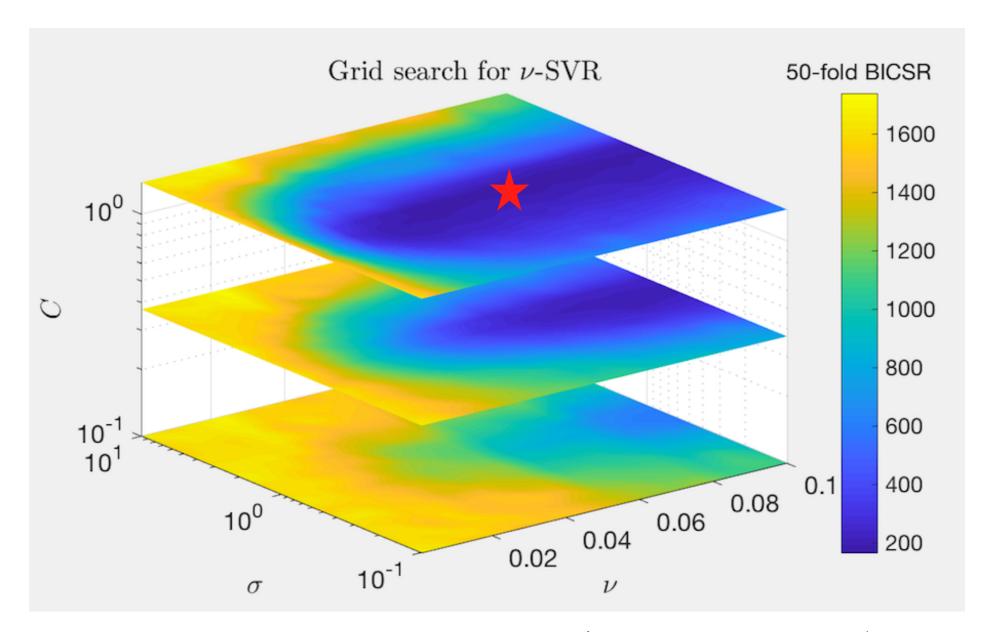
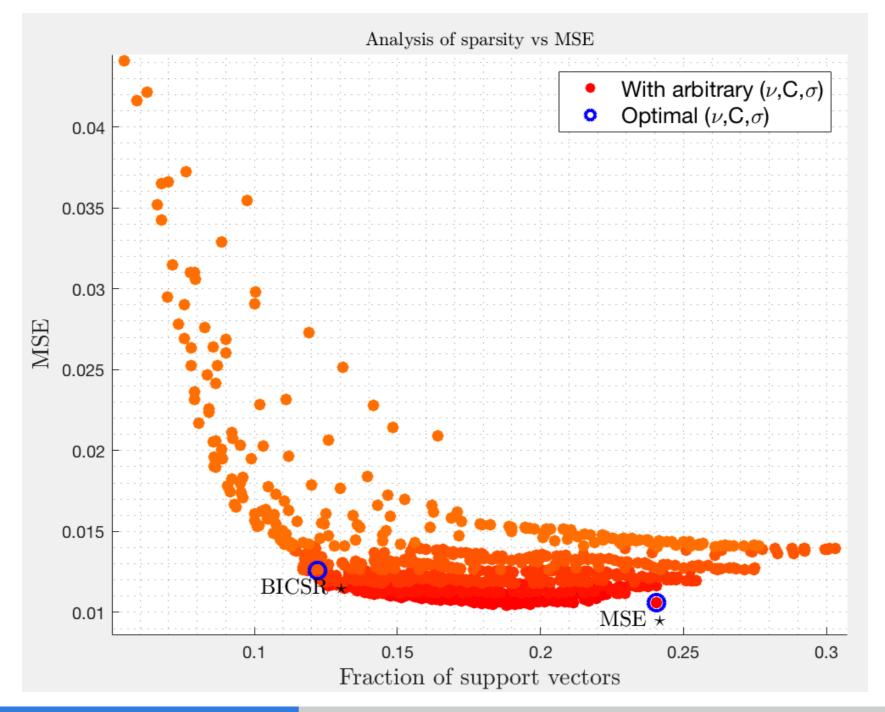
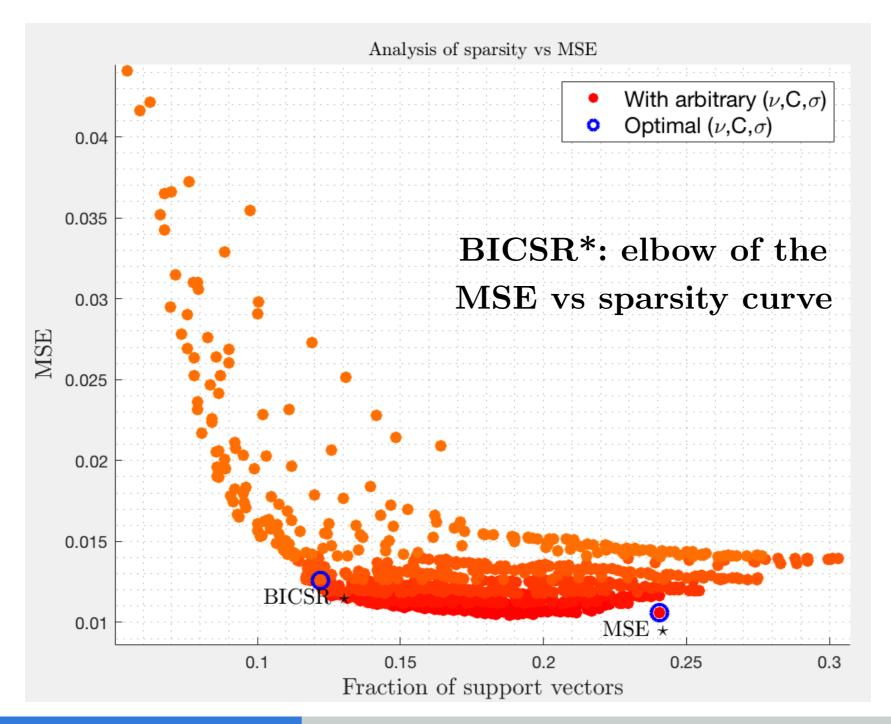


Figure: 50-fold cross-validation (0.75 training/test ratio)

- Tradeoff evaluation (artificial dataset)
  - Example for SVR (50 fold, 75 training/test ratio):



- Tradeoff evaluation (artificial dataset)
  - Example for SVR (50 fold, 75 training/test ratio):

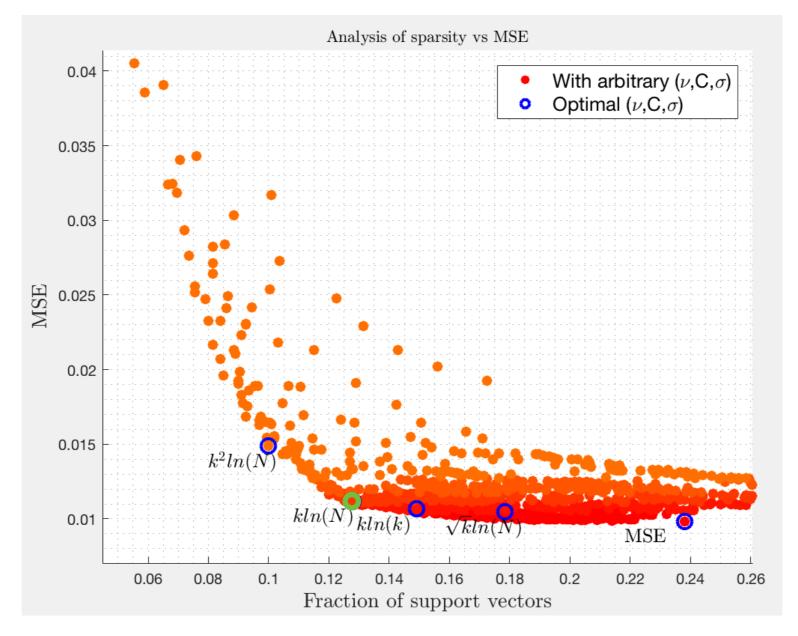


- Tradeoff evaluation (artificial dataset)
- Can we do better (different penalization)?

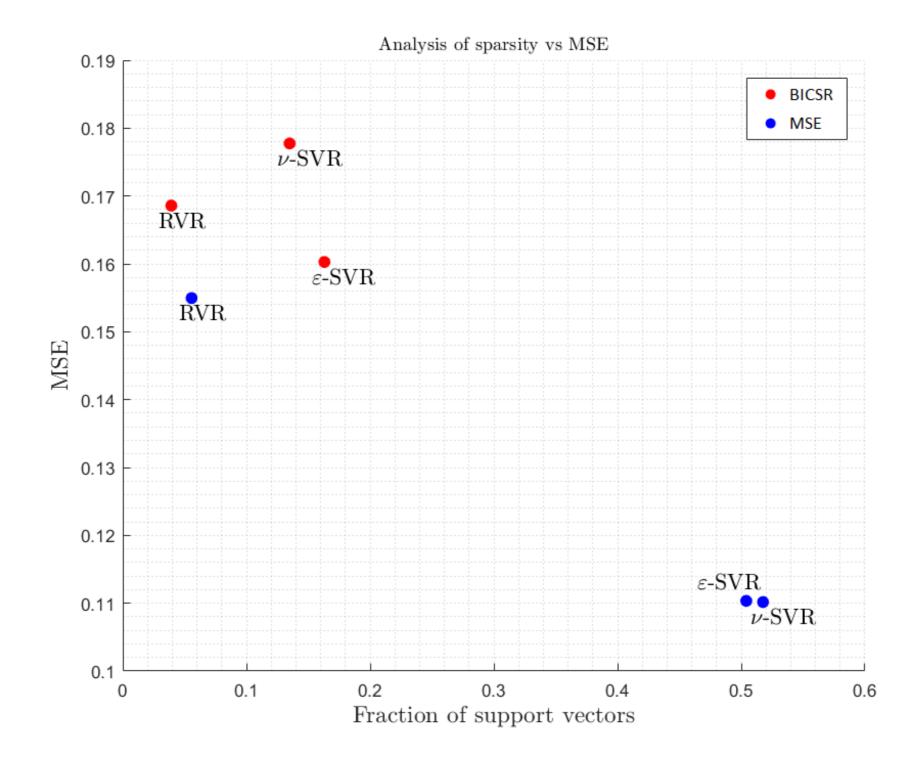
$$BICSR = \beta^{-1}N \cdot MSE + k \log N$$

- Tradeoff evaluation (artificial dataset)
- Can we do better (different penalization)?

$$BICSR = \beta^{-1}N \cdot MSE + k \log N$$



# ■ Model Comparaison (real dataset)



#### Conclusions

• BICSR seems to be a well-behaved sparse-regression metric (tradeoff between sparsity and performance)

• Even without sparsity penalization, RVR finds a fairly good compromise

most suited for fast predictions!

• SVR can be tuned to achieve either high sparsity or high regression performance

#### Other aspects:

- Behavior far from data
- Training cost
- Decision theory for predictions (predictive distribution)

#### Advanced Machine Learning

Thank you for your attention!