Some aspects of SVM Regression: an example for spectroscopic quantitative predictions

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Summary

• What are SVM?
  • SVM Regression
  • Criteria to optimize
  • The risk of overfitting
  • Two algorithms

• Fit non-linear spectroscopic data with SVM
  • Data set
  • Non-linearity issues
  • Spectroscopic pretreatments
  • X-Data compression
  • Training Set size
  • Comparison of algorithms

• Conclusions
What are SVM?

• Principle of Support Vector Machines
  • Supervised methods based on margins
  • Only a few samples are used for the calculation of the final model
    = samples defining the margins = support vectors

• How to cope with non-linearities
  • Non-linearities can be modeled thanks to data transformation into a kernel = similarity between samples
    • Gaussian kernel:
      \[ K(x_i, x_j) = e^{-\frac{\|x_i-x_j\|^2}{\sigma^2}} \]
  • Parameters to adjust: C, ε, σ²

Source: Eigenvector Research Inc.
Criteria to optimize

• Epsilon $\varepsilon$:
  • Has a direct effect on the size of the margin: a small epsilon leads to a tight margin (tighter fitting to the calibration set)
    • Directly correlated to the number of support vectors selected
    • Low impact on the error (on a ‘reasonable’ range)

Increase of epsilon

Y predicted, Y reference, Margins

Not a support vector anymore
Criteria to optimize

• **Sigma $\sigma^2$:**
  • Determines the degree of non-linearity of the model
    - Smaller sigma allows the SVM to represent stronger non-linearity
    - Larger sigma tends towards linear kernel behavior
      • Criterion that seems the more prone to cause overfitting (or underfitting)
      • Linked to the level of X values

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![Small sigma](image1.png)

![High sigma](image2.png)

Support vectors
Criteria to optimize

- **Cost C**: *penalty (or regularization) parameter*
  - High cost: errors very impactful, dangerous if outliers
  - Low cost: might lead to under-fitting

\[
\min \left( C \sum_{i=1}^{n} \xi_i + \frac{b^T b}{2} \right)
\]

With:
\[
\xi_i = \begin{cases} 
0 & \text{if } |y_i - \hat{y}_i| < \varepsilon \\
|y_i - \hat{y}_i| & \text{otherwise}
\end{cases}
\]

*b* – coefficients of the regression
Optimization map

Cross validation – mean squared error

Gamma fixed

Cross validation – mean squared error

Epsilon fixed

\[ \log_{10}(\text{cost}) \]

\[ \log_{10}(\epsilon) \]

\[ \log_{10}(\gamma) = \log_{10}(\sigma^{-2}) \]

Software: PLS Toolbox (Eigenvector Research Inc.)
**SVM Regression:** the risk of overfitting

- **Warning:** unproperly tuned, SVM can overfit very quickly!

Example: Y randomized: still possible to achieve good results on the calibration set

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**Software:** PLS Toolbox (Eigenvector Research Inc.)

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SVM Regression: 2 algorithms

- SVM-R (or SVR): minimization of the sum of the errors higher than epsilon

\[
\min \left( C \sum_{i=1}^{n} \xi_i + \frac{b^T b}{2} \right) \quad \text{With:} \quad \xi_i = \begin{cases} 
0 & \text{if } |y_i - \hat{y}_i| < \varepsilon \\
|y_i - \hat{y}_i| & \text{otherwise}
\end{cases}
\]

- LS-SVM: minimization of the sum of squared errors
  - All samples are support vectors

\[
\min \left( C \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 + \frac{b^T b}{2} \right)
\]
Summary

- **What are SVM?**
  - SVM Regression
  - Criteria to optimize
  - The risk of overfitting
  - Two algorithms

- **Fit non-linear spectroscopic data with SVM**
  - Data set
  - Non-linearity issues
  - Spectroscopic pretreatments
  - X-Data compression
  - Training Set size
  - Comparison of algorithms

- **Conclusions**
Data set

- Near Infrared spectroscopic data on raw meat. Three quantitative chemical results available: moisture content, fat content, protein content.

- Instrument: FOSS Tecator Infratec Food and Feed Analyzer
  - Range: 850-1050 nm

- Dataset
  - Training set: 158 samples
  - Test set: 35 samples
  - Cross-validation 2 blocks

Source: http://lib.stat.cmu.edu/datasets/tecator
Non-linearity issues

- Strong non-linearities: example of PLS linear modeling

Software: PLS Toolbox (Eigenvector Research Inc.)
Spectroscopic pretreatments

- 4 modalities tested: raw, D1, D2, SNV
- Strong impact of the pretreatment on the results with SVM-R

SVM are based on sample similarities, thus any perturbation should be corrected (e.g. scattering effect)

Software: PLS Toolbox (Eigenvector Research Inc.)
**X-data compression**

- Compression can be useful with spectroscopic data
  - Scores from PCA or PLS model used instead of spectra
  - Possibility to correct the scores with Mahalanobis distance (equivalent to scaling)
  - Careful not to select too many components to avoid overfitting

> In this particular example, results are globally better without compression. Compression should then not be automatically done, but investigated for each case.
Compression

Too many components can lead to overfit, especially with a correction from the Mahalanobis distance (normalization)

Y = Protein – PCA compression – 10 principal components
Scores corrected from the Mahalanobis distance

Y = Protein – PCA compression – 10 principal components
Non corrected scores

Software: PLS Toolbox (Eigenvector Research Inc.)
Compression

Example of an extreme case: PCA compression with 50 principal components

- Too many components combined with Mahalanobis correction might lead us to model noise

Software: PLS Toolbox (Eigenvector Research Inc.)

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**Training set size**

- How does the SVM perform with fewer training samples?
- Crop of the calibration set – down to 10% of the initial set. Test set identical.

Examples on moisture – strong non-linearities

- and on protein – weak non-linearity

➢ In this case, results acceptable with SVM up to 25% of the original calibration set (N = 40)
## Comparison of algorithms

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Algorithm</th>
<th>Pretreatment</th>
<th>N LVs</th>
<th>N SVs</th>
<th>Bias test</th>
<th>R² test</th>
<th>RPD test</th>
<th>SEP</th>
<th>SEP (%)</th>
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</thead>
<tbody>
<tr>
<td>fat</td>
<td>PLS</td>
<td>D1</td>
<td>3</td>
<td>-</td>
<td>-0.49</td>
<td>0.953</td>
<td>4.6</td>
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<td>19.4%</td>
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<td>D1</td>
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<td>1.06</td>
<td>0.996</td>
<td>9.3</td>
<td>1.37</td>
<td>10%</td>
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<tr>
<td>moisture</td>
<td>PLS</td>
<td>SNV</td>
<td>3</td>
<td>-</td>
<td>0.14</td>
<td>0.966</td>
<td>5.6</td>
<td>1.78</td>
<td>2.7%</td>
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<td>SNV</td>
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<td>0.965</td>
<td>4.9</td>
<td>0.62</td>
<td>3.3%</td>
</tr>
</tbody>
</table>

- SVM algorithms significantly better than PLS
- Even for protein content, which showed weak non-linearity

**Software:**
- SVM-R: PLS Toolbox (Eigenvector Research Inc.)
Comparison of algorithms

Fat PLS

Fat SVM-R

Fat LS-SVM

Moisture PLS

Moisture SVM-R

Moisture LS-SVM

Protein PLS

Protein SVM-R

Protein LS-SVM

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Conclusion

• SVM are very useful for non linear data
  • Much better results than PLS
  • Works also well for linear data!

• Efficient even with a low number of samples in the calibration set
  • In this particular study, satisfactory results obtained with 40 samples in the calibration set
  • Interesting alternative to ANN

• Careful however not to overfit!
Prestations et formation en
Analyse de données /
Chimiométrie /
Data Analytics

- Analyse exploratoire/ Data-mining
- Calibration spectroscopique
- Multivariate Process Control (MSPC)
- Multi-blocs / Fusion de données
- Plans d’Expériences

Merci pour votre attention!