Statistical learning and ensembling techniques for time-series-based model building

Maciej Ogorzałek\textsuperscript{1,2}
Christian Merkwirth\textsuperscript{1}

\textsuperscript{1}IT Department, Jagiellonian University, Kraków
\textsuperscript{2}AGH University of Science and Technology, Kraków
Given: A sample of input-output-pairs \((\vec{x}^\mu, y^\mu)\) with \(\mu = 1, \ldots, N\)
A functional dependence \(y(\vec{x})\) (maybe corrupted by noise)

Aim: Choosing a model (function) \(\hat{f}\) out of hypothesis space \(\mathcal{H}\)
close to true dependency \(f\) as possible

Classification \(f : \mathbb{R}^D \mapsto \{0, 1, 2, \ldots\}\) discrete classes
Regression \(f : \mathbb{R}^D \mapsto \mathbb{R}\) continuous output

Implementation usually via solution of an appropriate optimization problem:

- Matrix inversion in case of linear regression
- Minimization of a loss function on the training data
- Quadratic programming problem for SVMs
Validation and Model Selection

- **Generalization error**: How does the model perform on unseen data (samples)?
- Exact generalization error is not accessible since we have only limited number of observations!
- Training on small data set tends to **overfit**, causing generalization error to be significantly higher than training error
- Consequence of mismatch between the capacity of the hypothesis space $\mathcal{H}$ (VC-Dimension) (Vapnik-Cervonenkis) and the number of training observations
- **Validation**: Estimating the generalization error using just the given data set
  - Needed for choosing optimal model structure or learning parameters (step sizes etc.)
- **Model Selection**: Selecting the model with lowest (estimated) generalization error
- But estimation of generalization error is very unreliable on small data sets
Improving Generalization for Single Models

- Remedies:
  - Manipulating training algorithm (e.g. early stopping)
  - Regularization by adding a penalty to the loss function
  - Using algorithms with built-in capacity control (e.g. SVM)
  - Rely on criteria like BIC, AIC, GCV or Cross Validation to select optimal model complexity
  - Reformulate the loss function:
    - $\epsilon$-insensitive loss
    - Huber loss
    - SVM loss for classification
Are there any other methods to improve generalization error?
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Yes, by combining several individual models!
Ensemble: Averaging the output of several separately trained models

- Simple average
  \[ \bar{f}(\vec{x}) = \frac{1}{K} \sum_{k=1}^{K} f_k(\vec{x}) \]

- Weighted average
  \[ \bar{f}(\vec{x}) = \sum_{k} w_k f_k(\vec{x}) \text{ with } \sum_{k} w_k = 1 \]
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Error decomposition:

\[ e(\vec{x}) = (y(\vec{x}) - \bar{f}(\vec{x}))^2 \]
\[ \bar{e}(\vec{x}) = \frac{1}{K} \sum_{k=1}^{K} (y(\vec{x}) - f_k(\vec{x}))^2 \]
\[ \bar{a}(\vec{x}) = \frac{1}{K} \sum_{k=1}^{K} (f_k(\vec{x}) - \bar{f}(\vec{x}))^2 \]
\[ e(\vec{x}) = \bar{e}(\vec{x}) - \bar{a}(\vec{x}) \]
**Ensemble Methods**

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\]

Integrating over input space:

\[ E = \bar{E} - \bar{A} \]
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**Error decomposition:**

\[ e(\vec{x}) = (y(\vec{x}) - \bar{f}(\vec{x}))^2 \]

\[ \bar{\epsilon}(\vec{x}) = \frac{1}{K} \sum_{k=1}^{K} (y(\vec{x}) - f_k(\vec{x}))^2 \]

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\[ e(\vec{x}) = \bar{\epsilon}(\vec{x}) - \bar{a}(\vec{x}) \]

Interpretation:

- The ensemble generalization error is always smaller than the expected error of the individual models
- An ensemble should consist of well trained but diverse models
- An ensemble often outperforms the best constituting model

Integrating over input space:

\[ E = \bar{E} - \bar{A} \]
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How can we obtain models that have low generalization error (small \( \bar{E} \)), but are mutually uncorrelated (large \( \bar{A} \))? 

- Varying model structure (e.g. topology) 
- Exploiting the disadvantage of getting stuck in local minima: 
  - Varying initial conditions 
  - Varying parameters of the training procedure 
  - Using \( \epsilon \)-insensitive loss function 
- Train a large population of models 
- Applying resampling or sequencing techniques:
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How can we obtain models that have low generalization error (small $\bar{E}$), but are mutually uncorrelated (large $\bar{A}$)?

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- Train a large population of models
- Applying resampling or sequencing techniques:
  - Resampling: Generating new data sets by omitting or duplicating samples of the original data set. These techniques can be used to estimate generalization errors and for model construction
    - **Bootstraping** Generate bootstrap replicates by randomly drawing samples from training set
    - **Cross-Validation** Divide data set repeatedly in training and test part
    - **Bumping** Construct models on bootstrap replicates and choose best model on full data set
    - **Bagging** Bootstrap aggregation, create several models on bootstrap replicates and average these
    - **Boosting** Create sequence of models where training of next model depends on output of previous model
• Finesse: Efficiently reuse samples by combining training, validation and selection of models

• Additional benefit of reduced correlation between models

• Repeatedly partition data set randomly into two sample classes
  – Training set, used for training and stopping criteria
  – Test set, used only for accessing generalization error after model has been trained
• Finesse: Efficiently reuse samples by combining training, validation and selection of models
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• Repeatedly partition data set randomly into two sample classes
  – Training set, used for training and stopping criteria
  – Test set, used only for accessing generalization error after model has been trained
• Train population of (heterogenous) models, select best ones according to error on test set
• Repartition data set, taking care that test sets are mutually disjunct
• Combine best models of all partitionings to ensemble
• Optionally weight models according to the estimated generalization error on the total data set
Pros and Cons of Ensembles

Ensemble Methods

• Advantages
  – Straightforward extension of existing modeling algorithms
  – Almost fool-proof minimization of generalization error
  – Makes no assumptions on the structure of the underlying models
  – Simplifies the problem of model selection

• Disadvantages
  – Increased computational effort
  – Interpretation of ensemble is even harder than drawing conclusions from a single model
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Combining Heterogenous Models

• **Advantages**
  - Often one model type performs superior on the given data set
  - Probability of using an unsuited model type decreases
  - Inherent decorrelation even without manipulating data set or training parameters

• **Disadvantages**
  - Accessing the generalization performance of heterogenous models is even more difficult than for models of same type

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The ENTOOL toolbox for statistical learning is designed to make state-of-the-art machine learning algorithms available under a common interface.

- Allows construction of single models or ensembles of (heterogenous) models.
- Supports decorrelation of models by offering resampling techniques.
- Though primarily designed for regression, it is possible to construct ensembles of classifiers with ENTOOL.
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Requirements:
- Matlab (TM)

Operating systems:
- Windows
- Linux
- Solaris (limited)
• Each model type is implemented as separate class

• All model classes share common interface

• Exchange model types by exchanging constructor call

• Automatic generation of ensembles of models

• Models are divided into two brands:
  1. Primary models like linear models, neural networks, SVMs etc.
  2. Secondary models that rely on primary models to calculate output. All ensemble models are secondary models.
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Lifecycle of a model can be divided into three phases:
1. During construction, topology of the model is specified. The model can’t be used yet.
2. Model has now to be trained on some training data set \((\vec{x}_i, y_i)\)
3. After training, the model can be evaluated on new/unseen inputs \((\vec{x}_n)\)

Constructors should assign random default topologies in order to create uncorrelated models

It is possible to construct ensembles of ensembles
• Constructor syntax:
  
  `model = perceptron;` creates a MLP model with default topology
  `model = perceptron(12);` MLP model with 12 hidden layer neurons
  `model = ridge;` creates a linear model by ridge regression
Syntax

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- **Training syntax:**
  
  ```model = train(model, x, y, [], [], 0.05);``` trains model with $\epsilon$-insensitive loss of 0.05 on data set $(\vec{x}_i, y_i)$
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- **Evaluation syntax:**
  
  ```
  y_new = calc(model, x_new)  # evaluates the model on new inputs
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- **How to build an ensemble of models:**
  
  ens = crosstrainenensemble; will create an empty ensemble object  
  ens = train(ens, x, y, [], [], 0.05); calls training routines for several primary models and joins them into ensemble object
Adjusting class specific training parameters

- 5th argument when calling train specifies training parameters
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- 5th argument when calling `train` specifies training parameters
- Except topology, often training parameters have to be specified:

```python
tp = get(perceptron, 'trainparams')
error_loss_margin: 0.0100
decay: 0.0010
rounds: 500
mrate_init: 0.0100
max_weight: 10
mrate_grow: 1.2000
mrate_shrink: 0.5000
```
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- Assign new value: `tp.decay = 0.05`
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  ```
- **Assign new value:** `tp.decay = 0.05`
- **And give training parameters while training:**
  ```
  model = train(perceptron, x, y, [], tp, 0.05);
  ```
Ensemble constructor will train several models on dataset:

```plaintext
tp = get(crosstrainensemble, 'trainparams')

nr_cv_partitions:  8
frac_test:  0.2000
minimum_testsamples:  5
remove_worst:  0.3300
use_models:  0.8000
weight_models:  0
modelclasses:  6x3 cell
scaledata:  1
```
Specifying which Model Types to Ensemble

- Ensemble constructor will train several models on dataset:
  
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- Assign new value:
  
  ```matlab
  tp.modelclasses = {'perceptron', [], {}]; ... {'lssvm', [], {'function', 'RBF_kernel', 100, 2}}
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Primary Models Types

ares  Adaption of Friedman’s MARS algorithm
ridge  Linear model based on ridge regression with implicit LOO cross-validation for selecting optimal ridge penalty
perceptron  Multilayer perceptron with iRPROP+ training
perceptron2  Magnus Nørgaard’s single layer perceptron, trained with Levenberg-Marquart
prbfn  Shimon Cohen’s projection based radial basis function network
rbf  Mark Orr’s radial basis function code
vicinal  k-nearest-neighbor regression with adaptive metric
mpmr  Thomas Strohmann’s Mimimax Probability Machine Regression
lssvm  Johan Suykens’ least-square SVM toolbox
tree  Adaption of Matlab’s build-in regression/classification trees
osusvm  SVM code based on Chih-Jen Lin’s libSVM
vicinalclass  k-nearest-neighbor classification
**Ensemble Classes**

**ensemble**  Virtual parent class for all ensemble classes

**crosstrainensemble**  Ensemble class that trains models according to crosstraining scheme. Creates ensembles of decorrelated models.

**cvensemble**  Ensemble class that trains models according to crossvalidation/out-of-training scheme. Can be used to access OOT error.

**extendingsetensemble**  Boosting variant for regression.

**subspaceensemble**  Creates an ensemble of models where each single model is trained on a random subspace of the input data set.

**optimalsvm**  Wrapper that trains RBF osusvm/lssvm with optimal parameter settings ($C$ and $\gamma$)

**featureselector**  Does feature selection and trains model on selected subset
Application Examples

- Applications using ENTOOL
  - Nonlinear Regression of Skin Permeability
  - Sequence Analysis
- Molecular Graph Networks
  - Classification on NCI Data Set
  - Regression on KDD Challenge Data
Out-of-Train – CV for Ensembles

- **Out-of-Train Calculation** is combination of Cross Validation and Ensemble Averaging
- Inspired by Breiman’s Out-Of-Bag technique
- Construct ensemble of models on numerous train/test partitionings
- Don’t use test samples of each partition for model selection etc.
- OOT output for one sample of data set is average of all models where this sample was not in training set (out-of-train)
• **Out-of-Train Calculation** is combination of Cross Validation and Ensemble Averaging

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• Similar traditional CV, OOT tends to overestimate generalization error!

• Accounts for ensemble gain
Sensitivity Analysis for Regression

- Motivation: Determine variable importance with respect to prediction accuracy
- Might help uncovering causal relationships of underlying process
- Problem: Ensemble of heterogenous (nonlinear) models is even more difficult to analyze than single models
- Idea: Combine surrogate data method with OOT calculation
Sensitivity Analysis for Regression

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- Idea: Combine surrogate data method with OOT calculation

To determine importance of n-th variable:
- Create surrogate/replicate of the original input data set where values of n-th variable are permuted randomly to destroy information content
- Calculate OOT output for surrogate data set
- Compare errors of OOT output of surrogate and original data set
- If OOT error increases significantly, the n-th variable is important!
- Average importance over several surrogate data sets for same variable to smooth out noise
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• Problem: Ensemble of heterogenous (nonlinear) models is even more difficult to analyze than single models
• Idea: Combine surrogate data method with OOT calculation
• Retraining unnecessary, would mask importance of correlated inputs
• Uncovers linear and nonlinear relationships
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• 93 compounds described by 131 descriptors
• Ensemble of linear ridge models and k-nearest neighbor models
• Identified 8 descriptors by sensitivity analysis: 'Mass' 'Log P (oct/wat)' 'Cosmo' 'weinerPol'
  'logP(o/w)' 'SM 5.0R' 'TPSA' 'vol'
• Exhaustive check of all combinations of these descriptors leads to two final models:
  - 'Mass' 'logP(o/w)' 'Cosmo' with OOT error on training data set of 0.30 RMSE and on validation set of 0.31 RMSE
  - 'Mass' 'SM 5.0R' 'Log P (oct/wat)' with RMSE 0.28/0.28
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• Motivation: Determine importance of amino acid positions with respect to genotype-phenotype prediction accuracy

• Same idea as the sensitivity analysis for regression, but:
  – decrease in AUC (area under curve in ROC plot) instead of increase of MSE
  – random permutation of amino acids for each position
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- decrease in AUC (area under curve in ROC plot) instead of increase of MSE
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Application to HIV Receptor Interaction
- Data set of 355 samples with 63 AA positions
- Binary classification problem with 89 sequences that can use the CXCR4 receptor and 266 negatives
- Data set must be aligned first
- Ensemble of SVM, linear and k-NN classifiers
- Drawback: Quality of sensitivity analysis strongly depends on OOT prediction accuracy
- Pro: Method can be used universally for genotype-phenotype matching and other classification settings
• Reasonable prediction accuracy on original data
• OOT AUC of 0.91
Sequence Analysis cont.

- Reasonable prediction accuracy on original data
- OOT AUC of 0.91
- Only a few sequence positions seem to be relevant:

![ROC curve and position-specific AUC]
NCI Data Set

- DTP AIDS Antiviral Screen
- Total 42682 compounds (7 outtakes)
- Three classes:
  1. CA - Confirmed active 423
  2. CM - Confirmed moderate 1080 compounds
  3. CI - Confirmed inactive compounds
- No information about targets
- Random partition into training set of 35000 compounds and test set of 7682 compounds
- Ensemble of networks trained with classification loss
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![Output Histograms](https://via.placeholder.com/150)

- **Multiple modes of activity possible**
Results: Classification on NCI Data Set

ROC

Frac. false positives

Frac. true positives

Test Class CI
OOT Train Class CI
Test Class CM
OOT Train Class CM
Test Class CA
OOT Train Class CA
Results: Classification on NCI Data Set

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Results: Toxicity Prediction

- EPA Fathead Minow Acute Toxicity Data Set of 617 industrial organic chemicals
- Predicting experimental LC 50
- MGN with 8 feature nets of 2-9 layers
- 50 fold Cross-Validation with 10% test on 577 compounds

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\[ r^2 = 0.58 \]


- Predictive Toxicity remains difficult
Summary

- Ensemble methods for classification and regression
- ENTOOL - Ensemble toolbox for Matlab
- State-of-the-art machine learning techniques
- Variety of primary and secondary model types
- Out-of-Train technique for accessing generalization error
- Sensitivity Analysis for classification and regression
- Application to skin permeability
- Application to genotype-phenotype matching
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- Variety of primary and secondary model types
- Out-of-Train technique for accessing generalization error
- Sensitivity Analysis for classification and regression
- Application to skin permeability
- Application to genotype-phenotype matching
- Applicable to data sets of any size
- Classification of active/inactive compounds NCI Antiviral Screen
- Toxicity prediction as regression problem
• Krogh, Vedelsby Neural Network Ensembles, Cross Validation and Active Learning Advances in Neural Information Processing Systems 7, MIT Press 1995

• Peronne, Cooper When networks disagree: Ensemble methods for neural networks Neural Networks for Speech and Image Processing, Chapman Hall 1993

• Hastie, Tibshirani, Friedman The Elements of Statistical Learning Springer 2001

• Vapnik The Nature of Statistical Learning Theory Springer 1999

• Chih-Chung Chang, Chih-Jen Lin LIBSVM : a library for support vector machines Software available at http://www.csie.ntu.edu.tw/~cjlin/libsvm 2001

• Freund Short introduction to boosting 1999


• Domingos A unified bias-variance decomposition for zero-one and squared loss Proceedings of the Seventeenth National Conference on Artificial Intelligence , 2000

• Breiman Bagging Predictors . Machine Learning, 24, 1996