

Experiences and Lessons in Developing Machine Learning and Data Mining Software

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Talk at Chinese R Conference, November, 2013

Machine Learning and Data Mining Software

- Most machine learning and data mining works focus on developing algorithms
- Researchers didn't pay much attention to software
- This situation has caused some problems
 1. The deployment of new algorithms still involves some issues needed to be studied by researchers.
 2. Without further investigation after publishing papers, researchers don't know how their algorithms are used.



Machine Learning and Data Mining Software (Cont'd)

- Fortunately, the R community has been very active in developing packages for public use
- How to generate useful machine learning software for **practical industry use** is a difficult and challenging issue



Machine Learning and Data Mining Software (Cont'd)

- In this talk, I will share our experiences in developing LIBSVM and LIBLINEAR.
- LIBSVM (Chang and Lin, 2011):
One of the most popular SVM packages; cited around **15,000** times on Google Scholar
- LIBLINEAR (Fan et al., 2008):
A library for large linear classification; widely used in Internet companies (e.g., Google, Yahoo!, eBay)



Outline

- 1 How users apply machine learning methods
- 2 An example: support vector machines
- 3 Considerations in designing machine learning software
- 4 Discussion and conclusions



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Most Users aren't Machine Learning Experts

- In developing LIBSVM, we found that many users have **zero** machine learning knowledge
- It is **unbelievable** that many asked what the difference between training and testing is



Most Users aren't Machine Learning Experts (Cont'd)

- A sample mail

From:

To: `cjlin@csie.ntu.edu.tw`

Subject: Doubt regarding SVM

Dear Sir,

 sir what is the difference between testing data and training data?

- Sometimes we cannot do much for such users



Most Users aren't Machine Learning Experts (Cont'd)

- Fortunately, more people have taken machine learning courses
Also, companies hire people with machine learning knowledge
- However, these engineers are still **not** machine learning experts



How Users Apply Machine Learning Methods?

For most users, what they hope is

- Prepare training and testing sets
- Run a package and get good results

What we have seen over the years is that

- Users expect good results **right after** using a method
- If method A doesn't work, they switch to B
- **They may inappropriately use most methods they tried**



How Users Apply Machine Learning Methods? (Cont'd)

In my opinion

- Machine learning packages should provide some simple and **automatic/semi-automatic** settings for users

These settings **may not be the best, but easily give users some reasonable results**

- If such settings are not enough, users many need to consult with machine learning experts.

I will illustrate the first point by a procedure we developed for SVM



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Support Vector Classification

- **Training** data (y_i, \mathbf{x}_i) , $i = 1, \dots, l$, $\mathbf{x}_i \in R^n$, $y_i = \pm 1$
- Most users know that SVM takes the following formulation (Boser et al., 1992; Cortes and Vapnik, 1995)

$$\min_{\mathbf{w}, b} \quad \frac{1}{2} \mathbf{w}^T \mathbf{w} + C \sum_{i=1}^l \max(1 - y_i(\mathbf{w}^T \phi(\mathbf{x}_i) + b), 0)$$

- $\phi(\mathbf{x})$: **high dimensional**, use kernel

$$K(\mathbf{x}_i, \mathbf{x}_j) \equiv \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$$



Let's Try a Practical Example

- A problem from a user in astroparticle physics

| | | | | |
|-----|----------|----------|-----------|----------|
| 1 | 2.61e+01 | 5.88e+01 | -1.89e-01 | 1.25e+02 |
| 1 | 5.70e+01 | 2.21e+02 | 8.60e-02 | 1.22e+02 |
| 1 | 1.72e+01 | 1.73e+02 | -1.29e-01 | 1.25e+02 |
| ... | | | | |
| 0 | 2.39e+01 | 3.89e+01 | 4.70e-01 | 1.25e+02 |
| 0 | 2.23e+01 | 2.26e+01 | 2.11e-01 | 1.01e+02 |
| 0 | 1.64e+01 | 3.92e+01 | -9.91e-02 | 3.24e+01 |

- Training set: 3,089 instances

Test set: 4,000 instances



The Story Behind this Data Set

- User:
I am using libsvm in a astroparticle physics application .. First, let me congratulate you to a really easy to use and nice package. Unfortunately, it gives me astonishingly bad results...
- OK. Please send us your data
- I am able to get 97% test accuracy. Is that good enough for you ?
- User:
You earned a copy of my PhD thesis



Direct Training and Testing

- For this data set, direct training and testing yields 66.925% test accuracy
- But training accuracy close to 100%
- Overfitting occurs because some features are in large numeric ranges (details not explained here)



Data Scaling

- For SVM, features shouldn't be in too large numeric ranges
- Also we need to avoid that **some features dominate**
- A simple solution is to scale each feature to $[0, 1]$

$$\frac{\text{feature value} - \text{min}}{\text{max} - \text{min}}$$

There are **other** scaling methods

- For this problem, after scaling, **test accuracy is increased to 96.15%**
- **Scaling is a simple and useful step; but many users didn't know it**



Parameter Selection

- For the earlier example, we use

$$C = 1, \quad \gamma = 1/4,$$

where γ is the parameter Gaussian (RBF) kernel

$$K(\mathbf{x}_i, \mathbf{x}_j) = e^{-\gamma \|\mathbf{x}_i - \mathbf{x}_j\|^2}$$

- Sometimes we need to properly select parameters
- For another set from a user

Direct training and test

$$\text{Test accuracy} = 2.44\%$$

After proper data scaling

$$\text{Test accuracy} = 12.20\%$$



Parameter Selection (Cont'd)

- Use parameter from cross validation on a grid of (C, γ) values

Test accuracy = 87.80%

- For SVM and other machine learning methods, **parameter selection is sometimes needed**
⇒ but users may not be aware of this step



A Simple Procedure for Beginners

After helping many users, we came up with the following procedure

1. Conduct simple **scaling** on the data
2. Consider **RBF** kernel $K(\mathbf{x}, \mathbf{y}) = e^{-\gamma\|\mathbf{x}-\mathbf{y}\|^2}$
3. Use cross-validation to find the **best parameter** C and γ
4. Use the best C and γ to **train the whole** training set
5. Test



A Simple Procedure for Beginners (Cont'd)

- We proposed this procedure in an “SVM guide” (Hsu et al., 2003) and implemented it in LIBSVM
- From research viewpoints, this procedure is **not novel**. We never thought about submitting our guide somewhere
- **But this procedure has been tremendously useful.**
Now almost the standard thing to do for SVM beginners



Lessons in Designing an Algorithm

- The method **doesn't need to be the best all the time**
- A method
 1. reasonably good in accuracy
 2. general enough to cover some types of data, and
 3. not very sensitive to parametersis often the most convenient for users
- Random Forest (Breiman, 2001) is such an example



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Which Functions to be Included?

- The answer is simple: **listen to users**
- While we criticize users' lack of machine learning knowledge, they point out many useful directions
- Example: LIBSVM supported only **binary** classification in the beginning. From many users' requests, we knew the importance of **multi-class** classification
- There are many possible approaches for multi-class SVM. Assume k classes



Which Function to be Included? (Cont'd)

- - One-versus-the rest: Train k binary SVMs:

1st class vs. $(2, \dots, k)$ th class

2nd class vs. $(1, 3, \dots, k)$ th class

⋮

- One-versus-one: train $k(k - 1)/2$ binary SVMs
 $(1, 2), (1, 3), \dots, (1, k), (2, 3), (2, 4), \dots, (k - 1, k)$

- We finished a study in Hsu and Lin (2002), which is now highly cited.
- Currently LIBSVM supports **one-vs-one** approach



Which Function to be Added? (Cont'd)

- LIBSVM is among the first SVM software to handle multi-class data.
This helps to attract many users.
- Users help to identify what are useful and what are not.



One or Many Options

- Sometimes we received the following requests
 1. In addition to “one-vs-one,” could you include other multi-class approaches such as “one-vs-the rest?”
 2. Could you extend LIBSVM to support other kernels such as χ^2 kernel?
- Two extremes in designing a package
 1. **One** option: reasonably good for most cases
 2. **Many** options: users try options to get best results



One or Many Options (Cont'd)

- From a research viewpoint, we should include everything, so users can play with them
- But
 - more options \Rightarrow more powerful
 - \Rightarrow more complicated
- Some users have **no abilities to choose between options**
- For LIBSVM, we took the “one option” approach but made it easily extensible



Simplicity versus Better Performance

- This issue is related to “one or many options” discussed before
- Example: Before, our cross validation (CV) procedure is not **stratified**
 - Results less stable because data of each class not evenly distributed to folds
 - We now support stratified CV, but code becomes more complicated
- In general, we **avoid changes for just marginal improvements**



Simplicity versus Better Performance (Cont'd)

- An earlier Google research blog “Lessons learned developing a practical large scale machine learning system” by Simon Tong
- From the blog, “It is perhaps less academically interesting to design an algorithm that is **slightly worse in accuracy, but that has greater ease of use and system reliability**. However, in our experience, it is very valuable in practice.”
- That is, **a complicated method with a slightly higher accuracy may not be useful in practice**



Numerical Stability

- Many classification methods (e.g., SVM, neural networks) involve numerical methods (e.g., solving an optimization problem)
- Numerical analysts have a **high standard** on their code, but machine learning people do not
- **This situation is expected:**
If we carefully implement method A but later method B gives higher accuracy \Rightarrow Efforts are wasted
- We should improve the quality of numerical implementations in machine learning packages



Numerical Stability (Cont'd)

- Example: In LIBSVM's probability outputs, we need to calculate

$$1 - p_i, \quad \text{where} \quad p_i \equiv \frac{1}{1 + \exp(\Delta)}$$

- When Δ is small, $p_i \approx 1$
- Then $1 - p_i$ is a **catastrophic cancellation**
- Catastrophic cancellation (Goldberg, 1991): when subtracting two **nearby** numbers, the relative error can be large so **most digits are meaningless**.



Numerical Stability (Cont'd)

- In a simple C++ program with double precision,

$$\Delta = -64 \quad \Rightarrow \quad 1 - \frac{1}{1 + \exp(\Delta)} \text{ returns zero}$$

but

$$\frac{\exp(\Delta)}{1 + \exp(\Delta)} \text{ gives more accurate result}$$

- Catastrophic cancellation may be resolved by **reformulation**
- This example shows that some techniques can be applied to improve numerical stability



Legacy Issues

- The **compatibility** between earlier and later versions restricts developers to conduct certain changes.
- We can avoid legacy issues by some programming techniques
- Example: we chose “one-vs-one” as the multi-class strategy in LIBSVM.
- **What if one day we would like to use a different multi-class method?**



Legacy Issues (Cont'd)

- Earlier in LIBSVM, we did not make the trained model a public structure

Encapsulation in object-oriented programming

- User can call

```
model = svm_train(...);
```

but **cannot** directly access a model's contents

```
int y1 = model.label[1];
```

- We provide functions to get model information

```
svm_get_nr_class(model);
```

```
svm_get_labels(model, ...);
```

- **Then users are transparent to the internal change on multi-class methods**



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Software versus Experiment Code

- Many researchers now release experiment code used for their papers

Reason: experiments can be reproduced

- This is important, but **experiment code is different from software**
- Experiment code often includes messy scripts for **various settings** in the paper – useful for reviewers



Software versus Experiment Code (Cont'd)

- Software: for **general users**
One or a few reasonable settings with a suitable interface are enough
- Many are now willing to release their experimental code
Basically you clean up the code after finishing a paper
- But working on and maintaining high-quality software take **much more work**



Software versus Experiment Code (Cont'd)

- Reproducibility different from replicability (Drummond, 2009)
Replicability: make sure things work on the sets used in the paper
Reproducibility: ensure that things work **in general**
- **The community now lacks incentives for researchers to work on high quality software**



Research versus Software Development

Shouldn't software be developed by companies?

Two issues

- 1 Business models of machine learning software
- 2 Research problems in developing software



Research versus Software Development (Cont'd)

Business model

- Machine learning software are basically “research” software
- They are often called by some bigger packages
For example, LIBSVM and LIBLINEAR are called by R, Weka and Rapidminer through interfaces
- It is unclear to me what a good model should be



Research versus Software Development (Cont'd)

Research issues

- A good package involves **more than the core learning algorithm**
- There are many other research issues
 - Numerical algorithms and their stability
 - Parameter tuning, feature generation, and user interfaces
 - Serious comparisons and system issues
- These issues also need researchers
- Currently we lack a system to encourage researchers to study these issues



Conclusions

- From my experience, developing machine learning software is very interesting
- We have learned a lot from users in different application areas
- We should encourage more researchers and engineers in the community to develop high quality software



Acknowledgments

- All users have greatly helped us to make improvements
Without them we cannot get this far
- We also thank all our past group members

