Lecture 12:

Meta-Learning Methods

November 28, 2006

Meta-Learning

- The idea of meta-learning is to come up with some procedure for taking a learning algorithm and a fixed training set, and somehow repeatedly applying the algorithm to *different* subsets (weightings) of the training set or using *different* parameters/choices within the algorithm in order to get a large ensemble of machines.
- The machines in the ensemble are then *combined* in some way to define the final output of the learning algorithm (e.g. classifier)
- The hope of meta-learning is that it can "supercharge" a mediocre learning algorithm into an excellent learning algorithm, without the need for any fancy new algorithms!
- There is, as always, good news and bad news....
  - The Bad News: there is (quite technically) No Free Lunch.
  - The Good News: for many real world datasets, meta learning works very well.

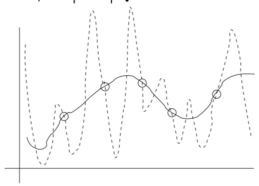
No Free Lunch

- David Wolpert and others have proven a series of theorems, known as the "no free lunch" theorems which, roughly speaking, say that *unless you make some assumptions* about the nature of the functions or densities you are modeling, no one learning algorithm can *a priori* be expected to do better than any other algorithm.
- In particular, this lack of clear advantage includes any algorithm and any meta-learning procedure applied to that algorithm. In fact, "anti-cross-validation" (i.e. picking the regularization parameters that give the *worst* performance on the CV samples) is a priori just as likely to do well as cross-validation. Without assumptions, random guessing is no worse than any other algorithm.
- So capacity control, regularlization, validation tricks and meta-learning cannot *always* be successful.

Generalization Error vs. Learning Error

- A key issue here is the difference between test error on a test set drawn from the same distribution as the training data (may contain duplicates) and *out of sample* test error.
- Remember back to the first class: learning binary functions. No assumptions == no generalization on out of sample cases. (The only way to learn is to wait until you have seen the whole world and memorize it.)
- Luckily, we *can* make some progress in real life. Why? Because the assumptions we make about function classes are often partly true.

x1	x2	x3	y
0	0	0	1
0	1	1	0
1	1	0	1
1	0	0	?
1	0	1	?



Meta-Learning Cafeteria 4

- Many meta-learning methods that work well in practice.
- We will review the three main ones:
  - Bagging: apply your algorithm to bootstrap datasets and average the predictions of the resulting ensemble.
  - Stacking: define a set of models by restricting the input to subsets of various sizes. Use LOO-CV to choose weights which blend these models.
  - Boosting: iteratively reweight your dataset, placing higher weights on the examples you are getting wrong. At each iteration, refit and add the result to your ensemble.
- Q: What do we apply meta-learing to?
  A: Weak models, e.g. decision stumps, linear regressors/classifiers.
- Meta-learning for classification/regression is well understood, but meta-learning for unsupervised learning is still an open problem.

Why does Meta-Learning Work? 5

- Either reduces variance substantially without affecting bias (bagging, stacking), or vice versa (boosting).
- All meta-learning is based on one of two observations:
  A) Variance Reduction: *If we had completely independent training sets* it always helps* to average together an ensemble of learners because this reduces variance without changing bias.
  B) Bias Reduction: For many simple models, a weighted average of those models (in some space) has much greater capacity than a single model (e.g. hyperplane classifiers, single-layer networks, Gaussian densities). So averaging models can often reduce bias substantially by increasing capacity; we can keep variance low by only fitting one member of the mixture at a time.

* see last page of notes

Bagging (Breiman 1994) 6

- Bagging $\equiv$ **b**ootstrap **agg**regation.
- Idea is simple. Generate B bootstrap samples from your original training set. Train on each one to get f_b. Now average them:

$$f_{bag} = \frac{1}{B} \sum_b f_b$$

- For regression, average predictions.
  For classification, average class probabilities
  (or take the majority vote if only hard outputs available).
- Bagging approximates the Bayesian posterior mean. The more bootstraps you use, the better, so use as many as you have time for.
- The size of each bootstrap sample is equal to the size of the original training set, but they are drawn *with replacement*, so each one contains some duplicates of certain training points and leaves out other training points completely.

Finite Bagging Can Hurt 7

- Bagging helps when a learning algorithm is good on average but *unstable* with respect to the training set.
- But if we bag a stable learning algorithm, we can actually make it worse. (For example, if we have a Bayes optimal algorithm, and we bag it, we might leave out some training samples in every bootstrap, and so the optimal algorithm will never be able to see them.)
- Bagging almost always helps with regression, but even with unstable learners it can hurt in classification.
  If we bag a poor & unstable classifier we can make it horrible.
- Example: true class = A for all inputs.
  Our learner guesses class A with probability 0.4 and class B with probability 0.6 regardless of the input. (Very unstable!).
  It has error 0.6.
  But if we bag it, it will have error 1.

Stacking (Wolpert 1990)

- In bagging, we created an ensemble of models by creating many synthetic training sets using the bootstrap.
- We can also create an ensemble of models in other ways, e.g. by restricting each model to look at only a subset of inputs, by trying the whole "kitchen sink" of regressors or classifiers (e.g. neural nets vs. logistic regression vs. naive bayes vs. KNN), by using a variety of regularization parameters, etc.
- In *stacked generalization* or *stacking* we try to find the best nonuniform weights to average our models together:

$$f_{stack}(x) = \sum_m w_m f_m(x)$$

- How should we set the weights? Using training error of each model? No! This will put too much weight on the most complex models.

Setting the Stacking Weights

- We estimate the optimal weights by setting them to minimize the average leave-one-out cross validation error:

$$w_m^* = \arg\min_w \sum_{i=1}^{N} \left[y_i - \sum_m w_m f_m^{-i}(x_i) \right]^2$$

where f_m^{-i} is the result of model m trained on all points except i.
- These weights can be found exactly using linear regression.
- This is like a generalization of model selection using LOO-CV. Previously we picked the best model and set $w_{mbest} = 1$ and all other $w_m = 0$. Now we are doing a smooth weighting.
- In more advanced stacking ideas, we can combine the models nonlinearly and use weights which depend on the input x. This is like a mixture of experts where we fit the gate using cross-validated training points instead of the usual training set.

Boosting (Shapire 1990)

- Probably one of the four most influential ideas in machine learning in the last decade, along with Kernel methods, Variational approximations, and Convex programming.
- In the PAC framework, boosting is a way of converting a "weak" learning model (behaves slightly better than chance) into a "strong" learning mode (behaves arbitrarily close to perfect).
- Very amazing theoretical result, but also led to a very powerful and practical algorithm (AdaBoost) which is used all the time in real world machine learning. Basic idea: divide and conquer.
- For binary classification with $y = \pm 1$.

$$f_{boost}(x) = \text{sign}\left[\sum_m \alpha_m f_m(x)\right]$$

where $f_m(x)$ are models trained with reweighted datasets D_m, and the weights α_m are non-negative.

AdaBoost Algorithm (Freund & Schapire 1997)

- Set initial observation weights $w_i = 1/N$. Set $m = 1$.
- Loop while ($err_m < .5$) {
  - Fit the base classifier to the training data weighted by w_i. This results in the m^{th} round classifier $f_m(x)$.
  - Compute $err_m = \sum_i w_i e_{mi} / \sum_i w_i$
    ($e_{mi} = 1$ if sign$[y_i] \neq$sign$[f_m(x_i)]$)
  - Set $\alpha_m = \frac{1}{2}\log[(1 - err_m)/err_m]$
  - Set $w_i \leftarrow w_i \exp[2\alpha_m e_{mi}]$
  - $m \leftarrow m + 1$

  }
- Final classifier is a weighted majority vote:

$$f_{boost}(x) = \text{sign}\left[\sum_m \alpha_m f_m(x)\right]$$

Some Intuitions about Boosting 12

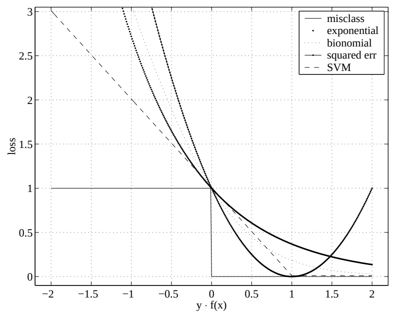
- At each round, boosting *increases* the weight on those examples the last classifier got wrong, and *decreases* the weight on those it got right. Thus, over time, it focusses on the examples that are consistently difficult and forgets about the ones that are consistently easy.
- The weight each intermediate classifier gets in the final ensemble depends on the error rate it achieved on its weighted training set at the time it was created.
- The reweighting over observations selected by boosting at each round is such that the previous classifier would perform at chance and so that the cross entropy between the previous weights and the new weights is minimized.

Boosting tries to minimize Exponential Loss 13

- An amazing fact, which helps a lot to understand how boosting really works, is that classification boosting is equivalent to fitting a greedy forward additive model using the following cost function:

$$\mathrm{cost}[y, f(x)] = \exp(-yf(x))$$

- This is called *exponential loss* and it is very similar to other kinds of loss, e.g. classification loss.



Forward Stagewise Additive Modeling 14

- Recall the additive model setup:

$$f_{add}(x) = \sum_m \alpha_m f_m(x; \theta_m)$$

- The overall function is a weighted sum of simpler functions, each with their own set of parameters.
  e.g.: hidden units in a MLP, wavelets, nodes in trees
- The optimization problem of finding the best $\{\alpha\}$ and $\{\theta\}$ simultaneously is usually extremely hard.
- But we can use a *greedy approximation*:
  - Initialize $f_0 = 0$.
  - for $m = 1 : M$ $\{$
    set $\alpha_m, \theta_m = \arg\min_{\alpha,\theta} \sum_{i=1}^N \mathrm{cost}[y_i, f_{m-1}(x_i) + \alpha f(x_i; \theta)]$
    set $f_m(x) = f_{m-1}(x) + \alpha_m f(x; \theta_m)$
    $\}$

Boosting as Forward Additive Modeling 15

- At each round of boosting we must minimize:

$$C = \sum_{i=1}^N \exp[-y_i(f_{m-1}(x_i) + \alpha_m f(x_i; \theta_m))]$$
$$= \sum_{i=1}^N w_i^m \exp[-\alpha_m y_i f(x_i; \theta_m)]$$

with respect to α_m and θ_m, where $w_i^m = \exp(-y_i f_{m-1}(x_i))$.

- The optimal function and weight are given by:

$$err_m = \sum_{i=1}^N w_i^m [y_i \neq f(x_i; \theta_m)] / \sum_i w_i^m$$
$$\theta_m^*(x) = \arg\min_\theta err_m$$
$$\alpha_m^* = \frac{1}{2} \log \frac{1 - err_m}{err_m}$$

Updating the observation weights

- Finally, we update our approximation to get

$$f_m(x) = f_{m-1}(x) + \alpha_m^* f(x; \theta_m^*)$$

- This sets the new weights:

$$\begin{aligned} w_i^{m+1} &= w_i^m \exp[-\alpha_m y_i f(x_i; \theta_m^*)] \\ &= w_i^m \exp[\alpha_m(2e_{mi} - 1)] \\ &= w_i^m \exp[2\alpha_m e_{mi}] \exp[-\alpha_m] \end{aligned}$$

  where the last factor of $\exp[-\alpha_m]$ just rescales all the weights uniformly, so we can drop it.

More on Exponential Loss

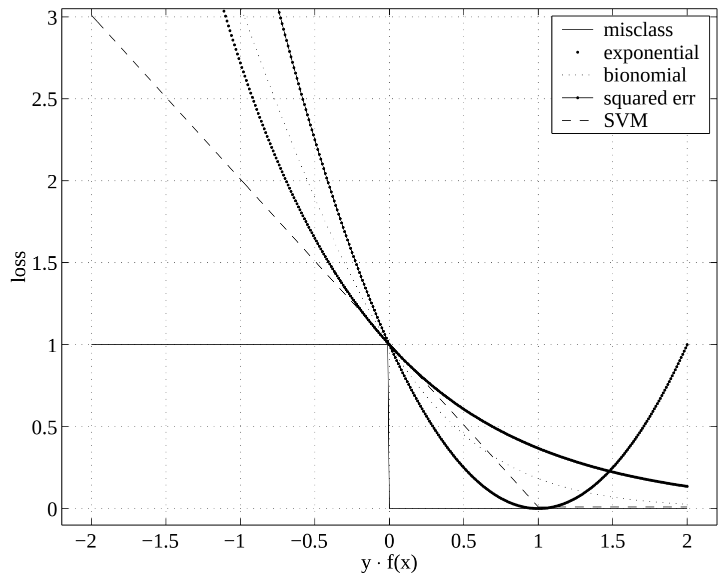
- Exponential loss is very similar to other classification losses.
- It is minimized by setting $f(x)$ to one half the log-odds:

$$f^*(x) = \frac{1}{2} \frac{Prob[y = 1|x]}{Prob[y = -1|x]}$$

  which means we can interpret $f(x)$ as the logit transform.
- Another loss function with the same population minimizer is the binomial negative log-likelihood:

$$-\log(1 + \exp(-2yf(x)))$$

- But binomial loss places less emphasis on the bad cases (high negative margin), and so it is more robust when data is noisy. Optimizing this is called *logit-Boost*.
- Boosting can also be thought of as trying to maximize a “margin” (like SVMs) but with a 1-norm constraint on the weights instead of a 2-norm constraint.



Variance Reduction by Averaging

- Here is an argument showing why averaging across independent training sets always reduces expected squared error:

$$\begin{aligned} e\bar{r}r_1 &= \sum_{x,y} p(x,y)\,(y - f(x|ts_1))^2 \\ e\bar{r}r &= \langle\langle \Big[y^2 - 2yf(x|ts) + f^2(x|ts) \Big] \rangle_{x,y} \rangle_{ts} = \langle e\bar{r}r_1 \rangle_{ts} \\ f_{meta}(x_{test}) &= \frac{1}{T} \sum_i f(x_{test}|ts_i) = \langle f(x_{test}|ts) \rangle_{ts} \\ e\bar{r}r_{meta} &= \sum_{x,y} p(x,y)(y - \langle f(x|ts) \rangle_{ts})^2 \\ &= \langle \Big[y^2 - 2y\langle f(x|ts) \rangle_{ts} + (\langle f(x|ts) \rangle_{ts})^2 \Big] \rangle_{x,y} \\ &\le \langle \Big[y^2 - 2y\langle f(x|ts) \rangle_{ts} + \langle f^2(x|ts) \rangle_{ts} \Big] \rangle_{x,y} \\ &\le e\bar{r}r \qquad \text{since } \langle f \rangle^2 \le \langle f^2 \rangle \end{aligned}$$