

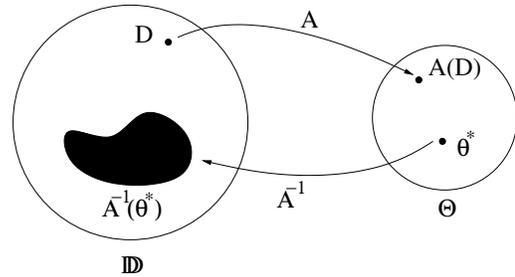
# Machine Teaching: An Inverse Problem to Machine Learning and an Approach Toward Optimal Education

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## Abstract

I draw the reader’s attention to machine teaching, the problem of finding an optimal training set given a machine learning algorithm and a target model. In addition to generating fascinating mathematical questions for computer scientists to ponder, machine teaching holds the promise of enhancing education and personnel training. The Socratic dialogue style aims to stimulate critical thinking.



## Of Machines

**Q:** *I know machine learning: What is machine teaching?*

Consider a “student” who is a machine learning algorithm, for example, a Support Vector Machine (SVM) or kmeans clustering. Now consider a “teacher” who wants the student to learn a target model  $\theta^*$ . For example,  $\theta^*$  can be a specific hyperplane in SVM, or the location of the  $k$  centroids in kmeans. The teacher knows  $\theta^*$  and the student’s learning algorithm, and teaches by giving the student training examples. Machine teaching aims to design the optimal training set  $D$ .

**Q:** *What do you mean by optimal?*

One definition is the cardinality of  $D$ : the smaller  $|D|$  is, the better. But there are other definitions as we shall see.

**Q:** *If we already know the true model  $\theta^*$ , why bother training a learner?*

The applications are such that the teacher and the learner are separate entities, and the teacher cannot directly “hard wire” the learner. One application is education where the learner is a human student. A more sinister “application” is security where the learner is an adaptive spam filter, and the “teacher” is a hacker who wishes to change the filtering behavior by sending the spam filter specially designed messages. Regardless of the intention, machine teaching aims to maximally influence the learner via optimal training data.

**Q:** *How is machine teaching an inverse problem to machine learning?*

One may view a machine learning algorithm  $A$  as a function mapping the space of training sets  $\mathbb{D}$  to a model space  $\Theta$ , see this figure:

Given a training set  $D \in \mathbb{D}$ , machine learning returns a model  $A(D) \in \Theta$ . Note  $A$  in general is many-to-one. Conversely, given a target model  $\theta^* \in \Theta$  the inverse function  $A^{-1}$  returns the set of training sets that will result in  $\theta^*$ . Machine teaching aims to identify the optimal member among  $A^{-1}(\theta^*)$ . However,  $A^{-1}$  is often challenging to compute, and may even be empty for some  $\theta^*$ . Machine teaching must handle these issues.

**Q:** *Isn’t machine teaching just active learning / experimental design?*

No. Recall active learning allows the learner to “ask questions” by selecting items  $x$  and asking an oracle for its label  $y$  (Settles 2012). Consider learning a noiseless threshold classifier in  $[0, 1]$ , as shown below.



To learn the decision boundary  $\theta^*$  up to  $\epsilon$ , active learning needs to perform binary search with  $\log(\frac{1}{\epsilon})$  queries. In contrast, in machine teaching the teacher only needs **two** examples:  $(\theta^* - \frac{\epsilon}{2}, -1)$ ,  $(\theta^* + \frac{\epsilon}{2}, +1)$ . The key difference is that the teacher knows  $\theta^*$  upfront and doesn’t need to explore. Note passive learning, where training items  $x$  are sampled *iid* uniformly from  $[0, 1]$ , requires  $O(\frac{1}{\epsilon})$  items.

**Q:** *So the teacher can create arbitrary training items?*

That is one teaching setting. Another setting is “pool-based teaching” where the teacher is given a pool of candidate items and can only select (or modify) those items. There are many other aspects of the teaching setting that one can consider: whether teaching is done in a batch or sequentially, whether the teacher has full knowledge of the learner, whether the learner is unsupervised or supervised, how to define training set optimality, and so on.

**Q:** *The optimal teaching data  $D$  can be non-iid?*

Yes, as the threshold classifier example shows. This is most noticeable when optimality of  $D$  is measured by its cardinality, but is in general true. It calls for new theoretical analysis methods for machine teaching, whereas traditional concentration inequalities based on *iid*-ness no longer apply.

**Q:** *Did you just invent machine teaching?*

No. What is new is our focus on tractable teaching computation for “modern” machine learners while generalizing the definition of optimality beyond training set cardinality. But there has been a long history of related work. The seminal notion of *teaching dimension* concerns the cardinality of the optimal teaching set (Goldman and Kearns 1995; Shinohara and Miyano 1991). However, the learner’s algorithm  $A$  was restricted to empirical risk minimization (specifically eliminating hypotheses inconsistent with training data). Subsequent theoretical developments can be found in e.g. (Zilles et al. 2011; Balbach and Zeugmann 2009; Angluin 2004; Angluin and Krikis 1997; Goldman and Mathias 1996; Mathias 1997; Balbach and Zeugmann 2006; Balbach 2008; Kobayashi and Shinohara 2009; Angluin and Krikis 2003; Rivest and Yin 1995; Ben-David and Eiron 1998; Doliwa et al. 2014). There are similar ideas in psychology, some of them can be found in the references in (Patil et al. 2014).

**Q:** *So you have a way to compute the optimal training set?*

This is in general still an open problem, but we now understand the solution for certain machine teaching tasks (Zhu 2013; Patil et al. 2014). Specifically, we restrict ourselves to batch teaching with full knowledge of the learning algorithm. The idea is as follows. Instead of directly computing the difficult inverse function  $A^{-1}(\theta^*)$ , we first convert it into an optimization problem:

$$\min_{D \in \mathbb{D}} \epsilon(D) \quad (1)$$

$$\text{s.t. } A(D) = \theta^*. \quad (2)$$

This is not the final formulation – it will evolve later.

**Q:** *OK. What is that  $\epsilon(D)$  objective?*

$\epsilon(D)$  is a “teaching effort function” which we must define to capture the notion of training set optimality. For example, if we define

$$\epsilon(D) = |D| \quad (3)$$

then we prefer small training sets. Alternatively, if we require the optimal training set to contain exactly  $n$  items we may define

$$\epsilon(D) = \mathbb{I}_{|D|=n} \quad (4)$$

where the indicator function  $\mathbb{I}_Z = 0$  if  $Z$  is true, and  $\infty$  otherwise. This teaching effort function is useful for designing human experiments as was done in (Patil et al. 2014). One can encode more complex notion of optimality with  $\epsilon(D)$ . For example, in teaching a classification task we may prefer that any two training items from different classes be clearly distinguishable. Here,  $D$  is of the form  $D = (x_1, y_1), \dots, (x_n, y_n)$ . We may define

$$\epsilon(D) = \sum_{i,j:y_i \neq y_j} \|x_i - x_j\|^{-1} \quad (5)$$

to avoid any near identical training items with different labels.

**Q:** *What is  $\mathbb{D}$  under your minimization in (1)?*

$\mathbb{D}$  is the search space of training sets. This is another design choice we must make. For example, we may decide upfront that in  $D$  we want  $n/2$  positive training examples and  $n/2$  negative ones, but the teacher can arbitrarily design each  $d$  dimensional feature vectors. The corresponding search space can be

$$\mathbb{D} = \{ \{ (x_i, y_i)_{1:n} \} \mid y_i = (-1)^i, x_i \in \mathbb{R}^d, i = 1 \dots n \}, \quad (6)$$

which is equivalent to  $\mathbb{R}^{nd}$ . Such a continuous search space is necessary for many standard optimization methods.

As another example, in pool-based machine teaching we are given a candidate item set  $S$ . The training set  $D$  must be a subset of  $S$ . Then  $\mathbb{D} = 2^S$ . Discrete optimization methods, such as those based on submodularity, may be applicable here (Krause and Golovin 2014; Iyer and Bilmes 2013; Bach 2013; Feige 1998; Krause and Guestrin 2005; Nemhauser, Wolsey, and Fisher 1978).

**Q:** *What about  $A(D)$  in (2)? Many machine learning algorithms do not have a closed-form solution w.r.t. the training set  $D$ .*

For some learners we are lucky to have a closed-form  $A(D)$ , and we can just plug in the closed-form expression. One example is ordinary least squares regression where  $A(D) = (X^T X)^{-1} X^T y$  with  $D = (X, y)$ . Another example is a Bayesian learner with a prior conjugate to  $D$ , where  $A(D)$  is simply the posterior distribution (Zhu 2013; Tenenbaum and Griffiths 2001; Rafferty and Griffiths 2010). Yet another example is a kernel density estimator where  $A(D)$  is written as a weighted sum of items in  $D$  (Patil et al. 2014).

But you are right. For most learners, there is no closed-form  $A(D)$ . Nonetheless, a very large fraction of modern machine learning algorithms are optimization-based. That means the learner itself can be expressed as an optimization problem of the form

$$\min_{\theta \in \Theta} R(\theta, D) + \Omega(\theta) \quad (7)$$

$$\text{s.t. } g(\theta) \leq 0, h(\theta) = 0. \quad (8)$$

Specifically,  $R(\theta, D)$  is the empirical risk function,  $\Omega(\theta)$  is the regularizer, and  $g, h$  are constraints when applicable. For these modern machine learners, we may replace  $A(D)$  in (2) by the machine learning optimization problem. This turns the original teaching problem (1) into a bilevel optimization problem:

$$\min_{D \in \mathbb{D}} \epsilon(D) \quad (9)$$

$$\text{s.t. } \theta^* \in \operatorname{argmin}_{\theta \in \Theta} R(\theta, D) + \Omega(\theta) \quad (10)$$

$$\text{s.t. } g(\theta) \leq 0, h(\theta) = 0. \quad (11)$$

In this bilevel optimization problem, the teaching objective (9) is known as the upper problem while the learning problem (10) is the lower problem.

**Q:** *Wait, I remember bilevel optimization is difficult.*

True, and solving (9) in general is a challenge. For certain convex learners, one strategy is to further replace the lower problem (10) by the corresponding Karush-Kuhn-Tucker conditions. In doing so, the lower problem becomes

a set of new constraints for the upper problem, and bilevel optimization reduces to a single level optimization problem.

**Q:** *I am still concerned. Constraints (2) and (10) looks overly stringent; it is like matching a needle in a haystack.*

I agree. The feasible sets can be exceedingly ill-formed. One way to address the issue is to relax the teaching constraint such that the learner does not need to exactly learn  $\theta^*$ . Indeed, the original teaching problem (1) is equivalent to

$$\min_{D \in \mathbb{D}} \mathbb{I}_{A(D)=\theta^*} + \epsilon(D). \quad (12)$$

Recall the indicator function is  $\mathbb{I}_Z = 0$  if  $Z$  is true, and  $\infty$  otherwise. We may relax the indicator by another “teaching risk function”  $\rho()$  with a minimum at  $\theta^*$ :

$$\min_{D \in \mathbb{D}} \rho(A(D), \theta^*) + \lambda \epsilon(D), \quad (13)$$

where  $\lambda$  is a weight that balances teaching risk and effort.  $\rho()$  would measure the quality of the learned model  $A(D)$  against the target model  $\theta^*$ . For example, a natural choice is  $\rho(A(D), \theta^*) = \|A(D) - \theta^*\|$ , which measure how close the learned model  $A(D)$  is to  $\theta^*$  in the parameter space with an appropriate norm. As another example, for teaching a classifier we may measure the teaching risk by how much  $A(D)$  and  $\theta^*$  disagree on future test data:

$$\rho(A(D), \theta^*) = \mathbb{E}_{x \sim P_X} \mathbf{1}_{A(D)(x) \neq \theta^*(x)} \quad (14)$$

where  $P_X$  is the marginal test distribution;  $\mathbf{1}_Z = 1$  if  $Z$  is true, and 0 otherwise; and we treat the models as classifiers.

We can then relax the bilevel optimization problem using the teaching risk function  $\rho()$  as follows:

$$\min_{D \in \mathbb{D}, \xi \in \Theta} \rho(\xi, \theta^*) + \lambda \epsilon(D) \quad (15)$$

$$\text{s.t. } \xi \in \operatorname{argmin}_{\theta \in \Theta} R(\theta, D) + \Omega(\theta) \quad (16)$$

$$\text{s.t. } g(\theta) \leq 0, h(\theta) = 0. \quad (17)$$

We can also bring the teaching effort function down as a constraint  $\epsilon(D) \leq B$  within some budget  $B$ .

**Q:** *There is still a glaring flaw: Can the teacher really have full knowledge of the learning algorithm?*

Good point. Under some circumstances this is plausible, such as when the learner is a robot and the teacher has its specifications. But when the learner is a human, we will rely on established cognitive models in the psychology and education literature. We will turn our attention to human learners in the next part of the article.

Before that, though, I briefly mention a setting where the teacher knows that the learning algorithm  $A$  is in a set  $\mathbb{A}$  of candidate learning algorithms, but not which one. As a concrete example,  $\mathbb{A}$  may be the set of SVMs with different regularization weights. Note that, given the same training data  $D$ , the learned model  $A(D)$  may be different for different  $A \in \mathbb{A}$ . The teacher knows that the learner is an SVM but doesn’t know its regularization weight.

A natural idea for this teaching setting is to “probe” the learner. A simple probing strategy for classification is as follows. Start by teaching the learner with an initial training set  $D_0$ . We assume the teacher cannot directly observe the resulting model  $A(D_0)$ . But the teacher can ask the learner to

make predictions on some test items  $X$  and observe the predicted labels  $A(D_0)(X)$ . The teacher can then eliminate all  $A' \in \mathbb{A}$  where  $A'(D_0)(X) \neq A(D_0)(X)$ . This procedure is repeated until  $\mathbb{A}$  is sufficiently reduced. Then the teacher finds the optimal training set for one of the remaining algorithms in  $\mathbb{A}$ . An open question is how to make combined probing and teaching optimal.

**Q:** *You generalized the notion of teaching optimality from  $|D|$  to arbitrary  $\epsilon(D)$ . Is there a theory for  $\epsilon(D)$  similar to teaching dimension?*

This is another open question.

## Of Humans

**Q:** *What can machine teaching do for humans?*

Machine teaching provides a unique approach to enhance education and personnel training. In principle, we can use machine teaching to design the optimal lesson for individual students.

**Q:** *There are already many intelligent computer tutoring systems out there, and MOOC – what is unique about machine teaching?*

Oversimplified, some existing education systems treat the human learner as a black-box function  $f(D)$ . The input  $D$  is educational intervention, e.g. which course modules to offer to the student. The output of  $f(D)$  is the student’s test score. The systems can make point evaluation of  $f$  at some input  $D$ , and aim to maximize  $f$  based on such evaluations, see e.g. (Lindsey et al. 2013). Being a black-box, the actual learning process of the student is not directly modeled.

In contrast, machine teaching explicitly assumes a *computational learning algorithm*, or a cognitive model,  $A$  of the student. Given educational intervention  $D$ , one may first compute the resulting cognitive state  $A(D)$ , which then leads to the observed test score via an appropriate teaching risk function  $\rho(A(D), \theta^*)$ . Thus, machine teaching treats the human learner as a “transparent box.” There is literature on such cognitive models for tutoring (Koedinger et al. 2013). Machine teaching’s focus is to explicitly compute the inverse  $A^{-1}$  to find the optimal lesson directly.

**Q:** *What is the advantage of machine teaching?*

The lesson will be optimal and personalized, given correct cognitive model of the student.

**Q:** *Isn’t “correct cognitive model” a strong assumption?*

True. Like many things in mathematics, the more conditions one posits, the stronger the result. Of course, empirically the quality of the lesson will depend on the validity of the cognitive model.

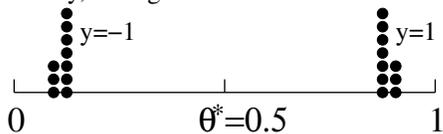
**Q:** *Do we have the correct cognitive model for education?*

Yes and no. For low level personnel training tasks such as improving the performance of human categorization, there are multiple well-established but competing cognitive models. On the other hand, accurate cognitive models for higher level education is still a work in progress. The latter is currently the major limit on the applicability of machine teaching to education. However, the community does have useful model fragments, and the machine teacher should take fully advantage of them.

**Q:** *So, is there indication that machine teaching works at all on humans?*

Yes. In (Patil et al. 2014) the authors studied a human categorization task, where participants learn to classify line segments as short vs. long. The assumed cognitive model was a limited capacity retrieval model of human learners similar to kernel density classifier. The teaching risk function  $\rho(\cdot)$  encodes the desire to minimize the expected future test error.

Machine teaching identified an interesting optimal training set: the negative training items are tightly clumped together, so are the positive training items, and the negative and positive items are symmetric but far away from the decision boundary, see figure below:



This solution resembles the toy example earlier; the larger separation between positive and negative items is due to a wide kernel bandwidth parameter in the cognitive model that fits noisy human behaviors.

Human participants indeed generalize better from this training set computed by machine teaching, compared to a control group who received *iid* uniformly sampled training sets. Both groups are tested on a test set consisting of a dense grid over the feature space. The group who received machine-teaching training set had an average test-set accuracy of 72.5%, while the control group 69.8%. The difference is statistically significant.

**Q:** *That's promising. Still, how do you know that you have the correct cognitive model? I remember you said there are other competing models.*

As is often said – all models are wrong, some are more useful. One may use the prior literature and data to come up with the best hypothesized model. They may be good enough for machine teaching to produce useful lessons.

While identifying such a model is an issue, it is also an opportunity – Strangely enough, another potential use of machine teaching in psychology is to adjudicate cognitive models.

**Q:** *Really? How can machine teaching tell which cognitive model is correct?*

Different cognitive models correspond to different learning algorithms. Call these algorithms  $A_1, \dots, A_m$ . Given a teaching target  $\theta^*$ , machine teaching can compute the optimal training set  $A_1^{-1}(\theta^*), \dots, A_m^{-1}(\theta^*)$  for each cognitive model, respectively. If previous result is any indication, these optimal training sets will each be non-*iid* and idiosyncratic.

We can then conduct a human experiment where we teach a participant using one of the  $m$  training sets, and test her on a common test set. Comparing multiple participants' test set performance, we identify the best training set, say  $A_j^{-1}(\theta^*)$ , among  $A_1^{-1}(\theta^*), \dots, A_m^{-1}(\theta^*)$ . This could lend weight to the  $j$ -th cognitive model  $A_j$  being the best cognitive model.

**Q:** *Tell me more about it.*

A variant is as follows. we conduct a different kind of human experiment: we ask the participant to be a teacher, and let the participant design a lesson intended to teach  $\theta^*$

to a human student. Let  $D$  be the lesson, i.e., the training data, that the participant comes up with. Assuming human teacher is (near) optimal, we can then compare  $D$  to  $A_1^{-1}(\theta^*), \dots, A_m^{-1}(\theta^*)$  to identify the best matching cognitive model  $A_j$ . We may then view  $A_j$  as what the human teacher assumes about the student. This is the strategy used in (Khan, Zhu, and Mutlu 2011).

## Coda

**Q:** *Now I am excited about machine teaching. What can I do?*

I call on the research community to study open problems in machine teaching, including:

**(Optimization)** Despite our early successes in certain teaching settings, solving for the optimal training data  $D$  is still difficult in general. We expect that many tools developed in the optimization community can be brought to bear on difficult problems like (15).

**(Theory)** Machine teaching originated from the theoretical study of teaching dimension. It is important to understand the theoretical properties of the optimal training set under more general teaching settings. We speculate that information theory may be a suitable tool here: the teacher is the encoder, the learner is the decoder, and the message is the target model  $\theta^*$ . But there is a twist: the decoder is not ideal. It is specified by whatever machine learning algorithm it runs.

**(Psychology)** Cognitive psychology has been the first place where machine teaching met humans. More studies are needed to adjudicate existing cognitive models for human categorization. Human experiments also call for new developments in machine teaching, such as the sequential teaching setting (Bengio et al. 2009; Khan, Zhu, and Mutlu 2011; McCandliss et al. 2002; Kumar, Packer, and Koller 2010; Lee and Grauman 2011; Cakmak and Lopes 2012; Pashler and Mozer 2013; Kobayashi and Shinohara 2009; Balbach and Zeugmann 2009). More broadly, psychologists have proposed cognitive models for many supervised and unsupervised human learning tasks besides categorization. These tasks form an ideal playground for machine teaching practitioners.

**(Education)** Arguably more complex, education first needs to identify computable cognitive models of the student. Existing intelligent tutoring systems are a good place to start: with a little effort, one may hypothesize the inner works of the student black-box. As a concrete example, at University of Wisconsin–Madison we are developing a cognitive model for chemistry education.

**(Novel applications)** Consider computer security. As mentioned earlier, machine teaching also describes the optimal attack strategy if a hacker wants to influence a learning agent, see (Mei and Zhu 2015) and the references therein. The question is, knowing the optimal attack strategy predicted by machine teaching, can we effectively defend the learning agent? There may be other serendipitous applications of machine teaching besides education and computer security. Perhaps you will discover the next one!

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