CSCI 4155/6505 (2016): Machine Learning

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Acknowledgements

These lecture notes have been inspired by several great sources, which I commend as further readings. In particular, Andrew Ng from Stanford University has several lecture notes on Machine Learning (CS229) and Artificial Intelligence: Principles and Techniques (CS221). His lecture notes and video links to his lectures are available on his web site (`http://robotics.stanford.edu/~ang`). Excellent book on the theory of machine learning are *Introduction to Machine Learning* by Ethem Alpaydin, 2nd edition, MIT Press 2010, and *Pattern Recognition and Machine Learning* by Christopher Bishop, Springer 2006. The standard book on RL is *Reinforcement Learning: An Introduction* by Richard Sutton and Andrew Barto, MIT press, 1998. The standard book for AI, *Artificial Intelligence: A Modern Approach* by Stuart Russell and Peter Norvig, 2nd edition, Prentice Hall, 2003, does also include some chapters on Machine Learning. Finally, the book by Kevin Murphy, Machine Learning: A Probabilistic Perspective is highly recommended for more in-depth studies.

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1 Introduction

1.1 The basic idea behind supervised ML

In the sense of its words, Machine Learning (ML) is the area that tries to build intelligent machines by defining a machine with specific operational abilities and training it with examples to perform specific tasks. This might sound like a niche area in science and you might wonder why there is now so much interest in this discipline, both academically and in industry. The reason is that ML is really about modeling data that provide the basis of advanced object recognition and data mining and is hence the analytical engine in areas such as data science, big data, data analytics and science in general.

ML has a long history with traces far back in time. One of the first recognized exciting realizations of the promise of learning machines came in the late 1950s and early 1960s with work like Arthur Samuel's self-learning checkers program and Frank Rosenblatt's perceptron. A second wave came in the 1980s and 90s with multilayer perceptrons and recurrent networks. And since 2006 we have a third wave of neural networks, that of deep learning which we will discuss more in this course.

ML is not restricted to neural networks. Indeed, the development of statistical machine learning and Bayesian networks has influenced the field strongly in the last 20 years and has been essential in much of its progress as well as in the deeper understanding of machine learning. This course will hence also introduce these more general ideas.

It is common and somewhat useful to distinguish three areas of machine learning, that of supervised learning, unsupervised learning, and reinforcement learning. Much of what is currently most associated with the success of ML is supervised learning, sometimes also called predictive learning. The basic task of supervised learning is that of taking as input a vector $\mathbf{x}$ of measurements, such as some medical measurements or robotic sensor data, and predicting an output value $\mathbf{y}$ such as the state of a patient's health or the location of obstacles. Note that we follow here a common notation of denoting a vector, matrix or tensor with bold faced letters, whereas we use regular fonds for scalars. We usually call the input vector a feature vector as the components of this are typically a set feature values of an object. The output could be also a multi-dimensional object such as a vector or tensor itself.

Mathematically we can denote the relations between the input and the output as a mapping function

$$y = f(\mathbf{x}), \tag{1.1}$$

where we consider here a single output value for convenience. The challenge for machine learning to know what the specific mapping function for a specific problem is. Machine learning has several approaches to deal with this. One approach that we will predominantly follow for much of the course is to define a general parameterized function

$$\hat{y} = \hat{f}(\mathbf{x}; \theta). \tag{1.2}$$

This formula describes that we make a parameterized hypothesis in which we specified a function $\hat{f}$ that depend on parameters to approximate the desired input-output relation. This function is called a **model**. We have indicated that this model is an approximation of the desired relation by using a hat symbol. However, we frequently drop this symbol when the relation is clear from the context, for example when the function contains parameters. The parameters are specified in this function by including the parameter as vector θ behind a semicolon in the function arguments. More appropriately, the formula defines a set of functions in the parameter space. A good solution represented by a point in this parameter space is an approximation that can be used for predicting output values (labels) $\hat{y}$ for specific input values.

We will later go one step further by considering the more general case when we might not be able to predict an exact value but at least the probability that a certain value will occur. Formulating ML learning in a probabilistic context has been most useful and provides us with the formalization that created the most insight into this field. In the stochastic framework we are then modelling a density function

$$p(\hat{y}|\theta). \tag{1.3}$$

For now we will follow the function approximation formalization, but we return to the probabilistic framework later.

1.2 Training, validating and testing

Coming up with the right parameterized approximation function is the hard problem in machine learning, and we will later discuss several choices. There are also methods to systematically develop the approximation function from the data, generally called non-parametric methods. However, we assume for now that we have a parameterized approximation function. The question is then how we determine good parameters. This is where the learning process comes in.

In supervised learning we must be given some examples of input-output relation from which we learn. We can think about these examples as given by a teacher. The teacher data called the **training set** are used to directly determine the parameters of the model. We can denote this training set as

$$\{\mathbf{x}(i), y(i)\}, \tag{1.4}$$

where the superscript i labels the specific training example. These indices are enclose in brackets to not confuse them with exponents.

There are different ways – usually called a training algorithm – to determine the parameters of a model. Let us illustrate this with an example where we assume we have a single input feature, x, and we hypotheses that the output y is linearly related to x. Mathematically we write this linear model as

$$\hat{y} = ax + b, \tag{1.5}$$

where a the slope of the linear function and b is the y-axis intercept or bias of this function. Using the training data to determine good parameters is also called regression in this context.

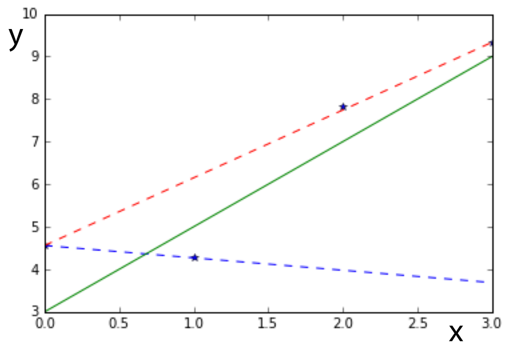


Fig. 1.1 A form of linear regression of data and cross-validation.

Let us illustrate an example regression procedure (there are different possible regression procedures) with the help of an example. For this we choose the true underlying model

$$y = 2x + 3 + \eta, \tag{1.6}$$

where η is a normal distributed random variable. We added this random addition to the perfect linear model to include right away a typical challenge in ML, that of having imprecise measurements and hence noisy training data. The other way to interpret the model is actually to accept the 'world' as stochastic and hence we are considering a stochastic model. In any case, from this model we chose some data points by sampling,

$$(0, 4.56)(1, 4.27), (2, 7.81), (3, 9.33) \tag{1.7}$$

We now make the assumption of a parameterized linear function

$$\hat{y} = ax + b, \tag{1.8}$$

with two parameters a and b, and use a simple method to determine the two parameters. As we have a linear equation with only two unknowns, we only need two data points to determine their values. Using the two first data points as emphtraining set we get

$$a = \frac{y^{(2)} - y^{(1)}}{x^{(2)} - x^{(1)}} = -0.29 \tag{1.9}$$

$$b = y^{(1)} - ax^{(1)} = 4.56 \tag{1.10}$$

This is not a very good agreement with the ideal values of $a = 2$ and $b = 3$. How about using the first and last data point as training set. The estimate of the y-intercept stays the same, but the slope estimation becomes $a = 1.59$ which is already much better.

But how would we know what the best solution is when we do not already know the solution? The answer is a procedure called **cross validation** where we use the data not used for training to validate the goodness of prediction on other data. Thus, the data not used directly to estimate the model parameters are called the **validation set**. We chose here to evaluate the goodness of the model with the mean square error (MSE) on the data not used for training

$$MSE = \frac{1}{N_{\text{val}}} \sum_{i=1}^{N_{\text{val}}} (\hat{y} - y)^2, \tag{1.11}$$

where N_{val} is the number of validation data. If we calculate the MSE for all possible data combinations we can choose as final estimation the estimation that leads to the smallest MSE of the unseen validation data points.

Cross validation is generally used to tune the **hyper-parameters**. Hyper-parameters are parameters of the learning algorithms. In our specific examples these are the choice of which data points to choose. Later we will discuss other learning algorithms that have hyper-parameter like a learning rate or the number of learning steps.

Finally, the ultimate test is using data that where not given to us during a learning phase to test the prediction of the model with the parameters that we estimated during the learning and cross-validation procedure. These data that are usually not given to the researchers during a training phase is recalled the **test set**. It is essential to be very clear about the differences between the training set, the validation set and the test set.

1.3 Unsupervised and reinforcement learning

Up to now we have discussed supervised learning where a teacher provides detailed examples of what the output of a machine should be. In **reinforcement learning** there is still some feedback from a teacher or the environment in the form of indicators that show how desirable the outputs of the learner is. This is often described as reward or punishment. However, the learning process requires some exploration as the learner must find the required action to attain a rewarding position. Such a learning requirement represents a common task in robotics and human learning, although a supervised learning system could be in itself a component of such a learning agenda, for example in the required vision system.

The last basic category of **unsupervised learning** is another important type of learning. This the of learning is more directly related to supervised learning except that the training data sets has no labels, That is, we are for example given a large data set of images but without detailed descriptions what the photographs represent. So one might ask how this can be of any use. However, there is a lot of information in the pictures itself as they give examples of how natural images look like or that there are usually edges and a certain distribution of colors. In other words, we can learn a lot about the statistics of the feature values from a large collection of unlabelled examples.

Some knowledge of the statistics of data is important to guide good representations of the data. We will se later that a good representation of data is a key element of solving mapping problems such as object recognition. Indeed, we can view the success of deep learning as the result of learning good layers of representations between the raw sensory input and the desired semantic space. It is therefore **representational learning** based on unsupervised and supervised learning that had build the foundation

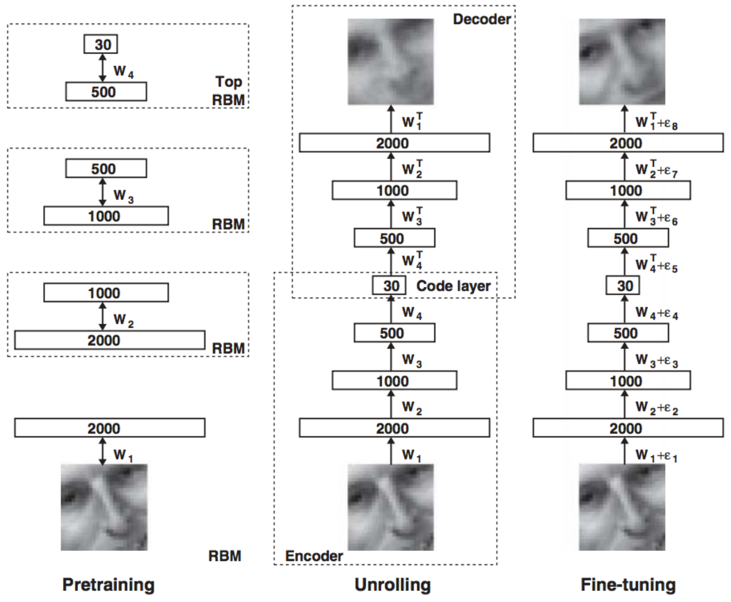
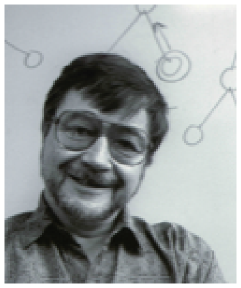


Fig. 1.2 A form of linear regression of data and cross-validation.

of much progress. For example, Figure 1.2 shows a famous work of Geoff Hinton and Ruslan Salakhutdinov published in Science 2006 of a neural network with several layers that transforms an input image to itself. At first it uses some unsupervised learning techniques that learns to reconstruct each input layer with a hidden layer. Such a network is called a **restricted Boltzmann machine**. Next we stack these layers on top of each other and train it like a supervised learning problem where the desired output (label) is the image itself. This is called an **autoencoder**. While the ability of translating an input image to itself might be questionable, the interesting part of such an autoencoder is that it has a number of representational layers in-between and that it has a bottleneck in the middle. This layer provides us with a **compressed representation** that is also interesting as it has been shown that it provides an interesting similarity measure between different inputs that can represent some semantic components. It is this kind of learning that provides a stream to more 'intelligent' processing.

1.4 Causal learning, overfitting and regression

I would like to close the introductory overview with on more concept that is central in machine learning. For this we go back to the supervised learning of repression. As mentioned previously finding the right parameterized function is somewhat difficult. There is an important area of **causal learning** that tries to provide specific probabilistic models of the components that provide the necessary foundations of the inference engine. Inference here means a system that can 'argue' about a solution in a probabilistic sense. Such systems fall generally in the domain of Bayesian learning, and we will include some introduction to this important systems in this course. Figure 1.3 shows an famous example form Judea Pearl, one of the inventors of this important modelling framework.



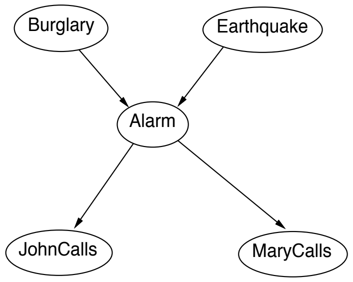


Fig. 1.3 Judea Pearl and causal modeling

Above we have discussed a case where we assumed a linear function, but regression with more general non-linear functions brings another level of challenges. An example of data that do not follow a linear trend is shown in Fig.1.4A. There, the number of transistors of microprocessors is plotted against the year each processor was introduced. This plot includes a line showing a linear regression, which is of course not very good. It is however interesting to note that this linear approximation shows some systematic deviation in some regional under and over estimation of the data. This systematic deviation or **bias** suggest that we have to take more complex functions into account. Finding the right function is one of the most difficult tasks, and there is not a simple algorithm that can give us the answer. This task is therefore an important area where experience, a good understanding of the problem domain, and a good understanding of scientific methods are required.

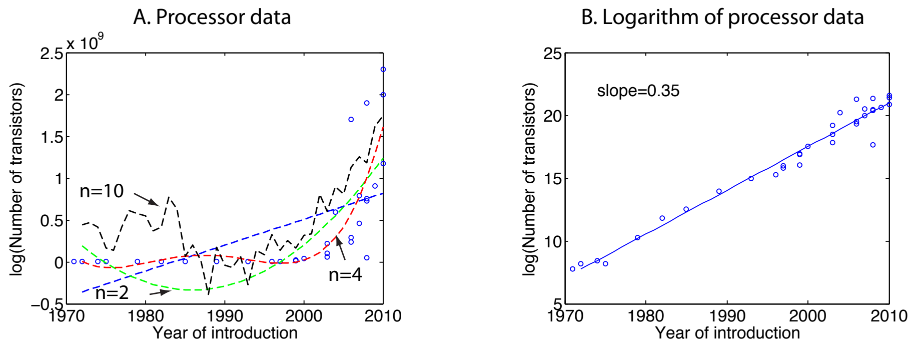


Fig. 1.4 Data showing the number of transistors in microprocessors plotted against the year they were introduced. (A) Data and some linear and polynomial fits of the data. (B) Logarithm of the data and linear fit of these data.

It is often a good idea to visualize data an various ways since the human mind is often quite advanced in 'seeing' trends and patterns. Domain-knowledge thereby very valuable as specialists in the area from which the data are collected can give important advice of or they might have specific hypothesis that can be investigated. It is also good to know common mechanisms that might influence processes. For example, the rate of change in basic growth processes is often proportional to the size of the system itself. Such an situation lead to exponential growth. (Think about why this is the case). Such situations can be revealed by plotting the functions on a logarithmic scale or the logarithm of the function as shown in Fig.1.4B. A linear fit of the logarithmic values is also shown, confirming that the average growth of the number of transistors in microprocessors is exponential.

But how about more general functions. For example, we can consider a polynomial of order n, that can be written as

$$y = \theta_0 x^0 + \theta_1 x^1 + \theta_2 x^2 + ... + \theta_n x^n \tag{1.12}$$

We can again use a regression method to determine the parameters from the data by minimizing the LMS error function between the hypothesis and the data. The LMS regression of the transistor data to a polynomials for orders $n = 2, 4, 10$ are shown in Fig.**??**A as dashed lines.

A major question when fitting data with fairly general non-linear functions is the order that we should consider. The polynomial of order $n = 4$ seem to somewhat fit the data. However, notice there are systematic deviations between the curve and the data points. For example, all the data between years 1980 and 1995 are below the fitted curve, while earlier data are all above the fitted curve. Such a systematic **bias** is typical when the order of the model is too low. However when we increase the order, then we usually get large fluctuations, or **variance**, in the curves. This fact is also called **overfitting** the data since we have typically too many parameters compared to the number of data points so that our model starts describing individual data points with their fluctuations that we earlier assumed to be due to some noise in the system. This difficulty to find the right balance between these two effects is also called the **bias-variance tradeoff**.

The bias-variance tradeoff is quite important in practical applications of machine learning because the complexity of the underlying problem is often not know. It then becomes quite important to study the performance of the learned solutions in some detail. A schematic figure showing the bias-variance tradeoff is shown in Fig.1.5. The plot shows the error rate as evaluated by the training data (dashed line) and validation curve (solid line) when considering models with different complexities. When the model complexity is lower than the true complexity of the problem, then it is common to have a large error both in the training set and in the evaluation due to some systematic bias. In the case when the complexity of the model is larger than the generative model of the data, then it is common to have a small error on the training data but a large error on the generalization data since the predictions are becoming too much focused on the individual examples. Thus varying the complexity of the data, and performing experiments such as training the system on different number of data sets or for different training parameters or iterations can reveal some of the problems of the models.

Deep neural networks are a form of high dimensional non-linear fitting function, and preventing overfitting is therefore a very important component in deep learning. Deep networks have many free parameters, and large data sets (big data) has therefor

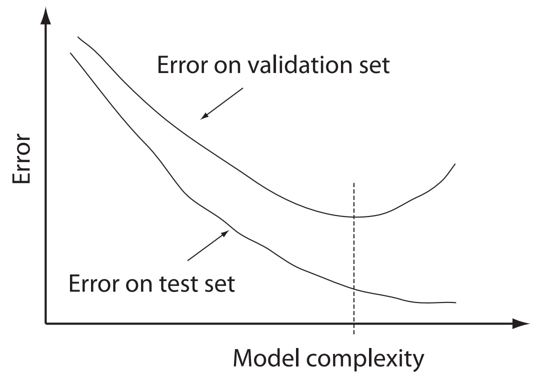


Fig. 1.5 Illustration of bias-variance tradeoff.

been important for the recent progress in this area in combination with other techniques to prevent overfitting such as a technique called dropout that we will discuss later. In general on can think about techniques to prevent overfitting as restricting the possible range of the parameters. Indeed, learning from data already represent providing information about the values of the parameters, and restricting such ranges further is a key element in machine learning. This are is generally discussed under the heading of **regularization**.

Machine learning methods are often easy to apply through application programs that implement these techniques. This is good news. However, a deeper understanding of the methods is necessary to make these applications and their conclusion appropriate. The machine learning algorithms will come up with some predictions, but if these predictions are sensible is important to comprehend and evaluate. Machine learning education needs therefore to go beyond learning how to run an application program, and this course thrives to find a balance between practical applications and their theoretical foundation.