Introduction to Machine Learning

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A possible definition of learning from Mitchell (1997):

A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E.

- **Task T**
  - *classification*: assigning one of \( k \) categories to a given input
  - *regression*: producing a number \( x \in \mathbb{R} \) for a given input
  - *structured prediction, denoising, density estimation, …*

- **Experience E**
  - *supervised*: usually a dataset with desired outcomes (*labels* or *targets*)
  - *unsupervised*: usually data without any annotation (*raw text, raw images, …*)
  - *reinforcement learning, semi-supervised learning, …*

- **Measure P**
  - *accuracy, error rate, F-score, …*
Deep Learning Highlights

- Image recognition
- Object detection
- Image segmentation
- Human pose estimation
- Image labeling
- Visual question answering
- Speech recognition and generation
- Lip reading
- Machine translation
- Machine translation without parallel data
- Chess, Go and Shogi
- Multiplayer Capture the flag
Figure 1.5, page 10 of Deep Learning Book, http://deeplearningbook.org.
Basic Machine Learning Settings

Assume we have an input of $\mathbf{x} \in \mathbb{R}^d$.

Then the two basic ML tasks are:

1. **regression**: The goal of a regression is to predict real-valued target variable $t \in \mathbb{R}$ of the given input.

2. **classification**: Assuming we have a fixed set of $K$ labels, the goal of a classification is to choose a corresponding label/class for a given input.
   - We can predict the class only.
   - We can predict the whole distribution of all classes probabilities.

We usually have a **training set**, which is assumed to consist of examples of $(\mathbf{x}, t)$ generated independently from a **data generating distribution**.

The goal of **optimization** is to match the training set as well as possible.

However, the goal of **machine learning** is to perform well on *previously unseen* data, to achieve lowest **generalization error** or **test error**. We typically estimate it using a **test set** of examples independent of the training set, but generated by the same data generating distribution.
Notation

- $a, \ a, \ A, \ A$: scalar (integer or real), vector, matrix, tensor
- $a, \ a, \ A$: scalar, vector, matrix random variable
- $\frac{df}{dx}$: derivative of $f$ with respect to $x$
- $\frac{\partial f}{\partial x}$: partial derivative of $f$ with respect to $x$
- $\nabla_x f$: gradient of $f$ with respect to $x$, i.e., $\left( \frac{\partial f(x)}{\partial x_1}, \frac{\partial f(x)}{\partial x_2}, \ldots, \frac{\partial f(x)}{\partial x_n} \right)$
Assume we have the following data, generated from an underlying curve by adding a small amount of Gaussian noise.
Linear Regression

Given an input value \( x \in \mathbb{R}^d \), one of the simplest models to predict a target real value is linear regression:

\[
f(x; w, b) = x^T w + b.
\]

The \( w \) are usually called \textit{weights} and \( b \) is called \textit{bias}.

Sometimes it is convenient not to deal with the bias separately. Instead, we might enlarge the input vector \( x \) by padding a value 1, and consider only \( x^T w \), where the role of a bias is accomplished by the last weight. Therefore, when we say “weights”, we usually mean both weights and biases.
Linear Regression

Assume we have a dataset of $N$ input values $x_1, \ldots, x_N$ and targets $t_1, \ldots, t_N$.

To find the values of weights, we usually minimize an error function between the real target values and their predictions.

A popular and simple error function is mean squared error:

$$\text{MSE}(w) = \frac{1}{N} \sum_{i=1}^{N} (f(x_i; w) - t_i)^2.$$ 

Often, sum of squares

$$\frac{1}{2} \sum_{i=1}^{N} (f(x_i; w) - t_i)^2$$

is used instead, because the math comes out nicer.

Figure 1.3 of Pattern Recognition and Machine Learning.
There are several ways how to minimize the error function, but in the case of linear regression and sum of squares error, there exists an explicit solution.

Assuming \( X \in \mathbb{R}^{N \times D} \) is a matrix of input values with \( x_i \) on a row \( i \), and \( t \in \mathbb{R}^N \) is a vector of target values, we are aiming to minimize

\[
\frac{1}{2} \| Xw - t \|^2 = \frac{1}{2} (Xw - t)^T (Xw - t).
\]

In order to find a minimum, we can inspect values where the derivative of the error function is zero.

\[
\nabla_w \frac{1}{2} (Xw - t)^T (Xw - t) = \nabla_w \frac{1}{2} (w^T X^T - t^T)(Xw - t)
\]
\[
= \frac{1}{2} X^T (Xw - t) + \frac{1}{2} X^T (Xw - t)
\]
\[
= X^T Xw - X^T t.
\]

For the derivative is therefore zero when \( X^T Xw = X^T t \), so when \( w = (X^T X)^{-1} X^T t \).
### Linear Regression

**Input:** Dataset \( \mathbf{X} \in \mathbb{R}^{N \times D}, \mathbf{t} \in \mathbb{R}^N \).

**Output:** Weights \( \mathbf{w} \in \mathbb{R}^D \) minimizing MSE of linear regression.

- \( \mathbf{w} \leftarrow (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{t} \).

The algorithm has complexity \( O(ND^2) \), assuming \( N \geq D \).

Note that there exist better solutions which do not require the \( (\mathbf{X}^\top \mathbf{X})^{-1} \) to exist (i.e., they solve directly the \( \mathbf{X}^\top \mathbf{X} \mathbf{w} = \mathbf{X}^\top \mathbf{t} \) equation), but they have the same complexity.
Linear Regression Example

Assume our input vectors comprise of $\mathbf{x} = (x^0, x^1, \ldots, x^M)$, for $M \geq 0$.

Figure 1.4 of Pattern Recognition and Machine Learning.
To plot the error, the root mean squared error $\text{RMSE} = \sqrt{\text{MSE}}$ is frequently used.

The displayed error nicely illustrates two main challenges in machine learning:

- underfitting
- overfitting

Figure 1.5 of Pattern Recognition and Machine Learning.
We can control whether a model underfits or overfits by modifying its capacity.

- representational capacity
- effective capacity

Figure 5.3, page 115 of Deep Learning Book, http://deeplearningbook.org
Linear Regression Overfitting

Note that employing more data also usually alleviates overfitting (the relative capacity of the model is decreased).

Figure 1.6 of Pattern Recognition and Machine Learning.
Regularization in a broad sense is any change in a machine learning algorithm that is designed to reduce generalization error but not necessarily its training error.

$L_2$ regularization (also called weighted decay) penalizes models with large weights:

$$\frac{1}{2} \sum_{i=1}^{N} (f(x_i; w) - t_i)^2 + \frac{\lambda}{2} ||w||^2$$

Figure 1.7 of Pattern Recognition and Machine Learning.
Regularizing Linear Regression

In matrix form, regularized sum of squares error for linear regression amounts to

$$\frac{1}{2} \|Xw - t\|^2 + \frac{\lambda}{2} \|w\|^2 = \frac{1}{2} (Xw - t)^T (Xw - t) + \frac{\lambda}{2} w^T w.$$ 

When repeating the same calculation as in the unregularized case, we arrive at

$$(X^T X + \lambda I)w = X^T t,$$

where $I$ is an identity matrix.

**Input:** Dataset $(X \in \mathbb{R}^{N \times D}, t \in \mathbb{R}^N)$, constant $\lambda \in \mathbb{R}^+$.  
**Output:** Weights $w \in \mathbb{R}^D$ minimizing MSE of regularized linear regression.

- $w \leftarrow (X^T X + \lambda I)^{-1} X^T t$. 
Choosing Hyperparameters

Hyperparameters are not adapted by the learning algorithm itself.

Usually a validation set or development set is used to estimate the generalization error, allowing to update hyperparameters accordingly. If there is not enough data (well, there is always not enough data), more sophisticated approaches can be used.

So far, we have seen two hyperparameters, $M$ and $\lambda$. 

Figure 1.8 of Pattern Recognition and Machine Learning.