<summarized from 11/25/18 meeting: Madhav, Abhijin, Srini>

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# Possible directions using machine learning techniques

## Artificial Neural Networks

## Transfer Learning

Machine learning (ML) algorithms typically perform well when the quantity and quality of training samples is high. However, coming up with data points is hard for the problem at hand; identifying sites infested by the target species is resource intensive. Also, seasonality, cloud cover and other factors can add to the challenges by restricting the number of usable satellite. A natural question to ask is, can we leverage a learner meant for a different but related problem? This learner might have been used to identify the presence of some other plant or to identify under a different class of inputs? Under these circumstances one resorts to transfer learning (TL), a design methodology in ML that enables one to transfer the knowledge learnt in one task (referred to as source task) to be transferred to other tasks (target tasks) (Pan, Yang, & others, 2010).

TL capitalizes on the fact that ML algorithms typically take a layered approach for learning (particularly deep learners). For images, it is observed that the initial layers extract low level features such as edges, changes in color, or gradient in temperature, while the middle layers might perform complex tasks of finding the correlation among the feature from different modalities with the higher layers performing task-specific functions such as defining classification rules or determining parameters of the prediction model. Although the distribution of the data might differ, the feature extraction process and the data modelling aspect of the layers would generally remain the same for the source and target. In cases where the target lacks labels but the tasks remain the same as the source, one could learn a mapping between the target and the source which then enables one to employ the labels available in the source domain. TL is also helpful when we consider tasks with insufficient training data. During the training phase, one could employ pre-trained feature extraction layers and augment the correlation capturing capability learned in the source domain to the available training data and then fine tune the task-specific learning functionality. The use of pre-trained layers allows one to invest precious training data for learning higher level functionalities. Utilizing the feature extraction functionality implies that all the training data can be utilized only for task-specific layers.

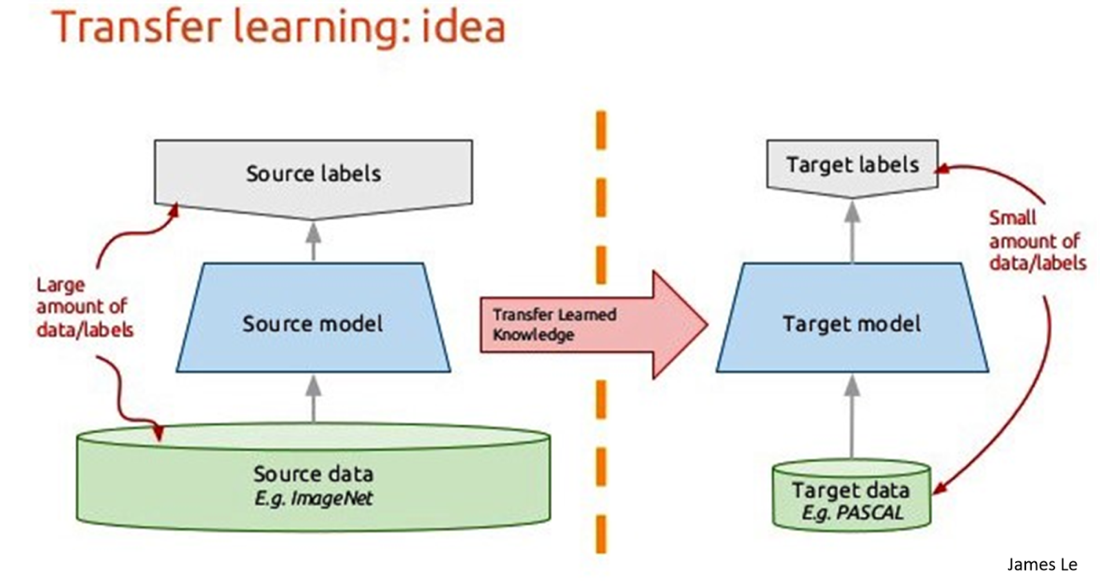


Figure 1. A schematic of transfer learning. Courtesy: William Vorhies (https://www.datasciencecentral.com).

## Combining data-driven models with theory-based models

Increasing availability of high-quality data and high-performance computing methods, have fueled the development of techniques such as deep learning. However, largely, these techniques are agnostic to underlying theory or understanding of the phenomenon under study. Mechanistic models, which are developed on the basis of fundamental of years of experience are not taken into account. It is natural that researches have eventually realized that the potential of combining these two paradigms of computational models for understanding complex phenomena. In this regard, two bodies of work have emerged in recent years, though the general concept has been around for a long: Theory-guided machine learning and the abduction loop. The integrated system has the following advantages: (i) Greater **consistency** as it respects known or accepted physical relationships between variables; (ii) **generalizability** allowing the user to make educated guesses under scarcity of data; and (iii) ability to evaluate **counterfactual** scenarios. For our study, potentially, these concepts can help create robust models under data inadequacy, guide data exploration, avoid overfitting, and help evaluate various intervention strategies.

### Theory-guided machine learning

Models based on scientific knowledge represent relationships between variables, for example, temperature and diapause. These are empirically proven, deduced from first principles or widely accepted by domain experts. Unlike these “theory-based” models, data-driven models use a set of training examples to learn a model that can automatically extract relationships between the input and output variables. Combining theory-based models with current data-driven models enables overcome many shortcomings of either methods. This has been demonstrated in a number of works concerning physical processes in domains such as hydrology and computational chemistry, and has been summarized in a survey (Karpatne et al., 2017). The survey describes the advantages and disadvantages of both modeling paradigms. More importantly, it clearly describes methods (with use cases) to fuse theory-based models with data-driven methods.

### Abduction loop (for informing field surveys)

Abduction is an inference approach that uses data and observations to identify plausible (preferably, best) explanations for phenomena (Peirce, Hartshorne, Weiss, & Burks, 1960). One-step abduction first generates data through experiments or observations. Then, data analysis consists of searching for patterns and generalizing these into phenomena, which is an inductive step. These results are used to formulate hypotheses based on theories whose purpose is to explain the data. Hypotheses may exist (from a previous loop) or may be proposed in this step, and can be removed (e.g., via falsification). Multiple candidate theories may be posed for a given phenomenon. Multi-agent models and mechanistic models of plant growth and response to ecological factors are candidate models at this stage. The best explanation, or hypothesis/theory appraisal, is the process of identifying the best explanation for the phenomenon; this includes hypothesis falsification. This stage can potentially identify gaps in data and guide surveys. Finally, the last step in an iteration is to determine what to do next, in terms of designing new experiments. The iterative process may terminate for any number of reasons; e.g., a best  
explanation has been found.

**References**

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**NWO research project page:** <https://www.nwo.nl/en/research-and-results/research-projects/i/30/20030.html>