Multi-Objective Regression for HEP

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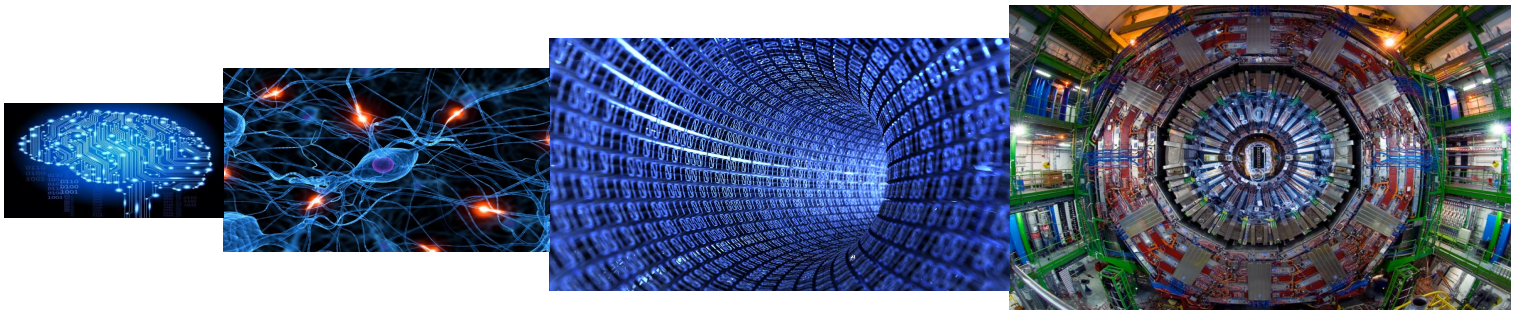


IML WG Meeting

Jan 18, 2016

Outline

- Classification
- Single-objective regression
- Multi-objective regression
- Applications

Classification

Classification

Train learning models to assign objects into discrete classes

- Cats, Dogs, Jets, Higg Bosons

With a machine learning algorithm

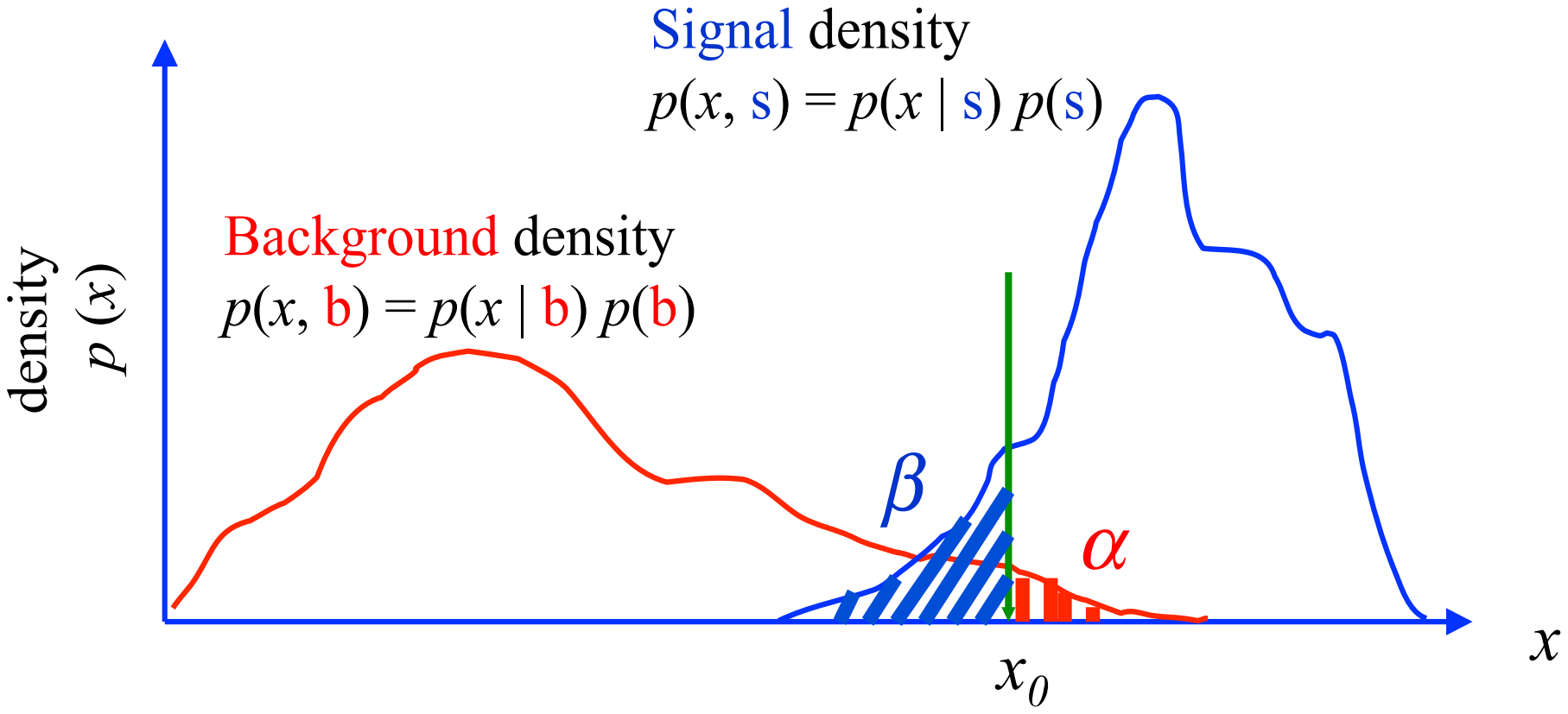
- Decision tree, random forest, neural network etc.

Classification

That minimizes some type of Loss function L

- In classification, you want to achieve maximum separation among classes

Classification Theory



Optimality criterion: minimize the error rate, $\alpha + \beta$

Function Estimation

Function Estimation

- Given enough data, estimate a function?
- Problem posed by Gauss (1805): estimate comet's trajectory from observations
- Solution: minimize difference between measurements and predictions by varying model parameters

Regression

- Inputs:
  - Training examples $\{<x^{(i)}, y^{(i)}>\}$ of unknown function f. $x^{(i)}, y^{(i)}$
- Output:
  - hypothesis that best approximates target function f

Regression

Modify evaluation criterion in the induction algorithm

– from maximum separation gain

– to minimal variance

Single-Target Estimation

Single-Objective Regression

Train learning model to estimate a single function target or "objective"

- Ex. photon energy/muon momentum

With a machine learning algorithm

- Decision tree, random forest, neural network etc.

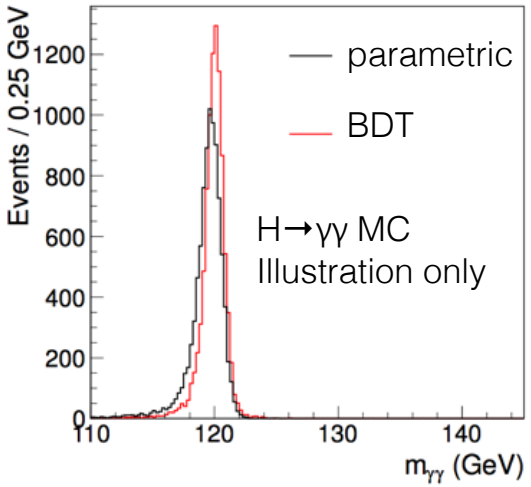
Photon Energy

Single Target Example:

Inputs: EM shower information, photon coordinates, median event energy

Target Output: $E_{MEASURED}/E_{TRUE}$

~10-30% improvement in resolution



Multi-Objective Regression

Multi-Objective Regression

- Problem requires simultaneous estimate of multiple functions or "targets"
  - May be additionally correlated
    - N single-target models are not as optimal for this problem (lingo: "multi-task" learning)
    - And more cumbersome.
- Train single model to simultaneously predict all targets

Applicable Models

- Methods:
  - Regression decision trees
  - Decision rules
  - Decision rule ensembles
  - Random forest
  - Neural networks…
- Trade-offs:
  - accuracy, model size, interpretability

Applications

Multi-objective Example

In HEP, this can be a transformation between two different classes of objects or learning to predict multiple parameters simultaneously

X input variables {a, b, c, d…}

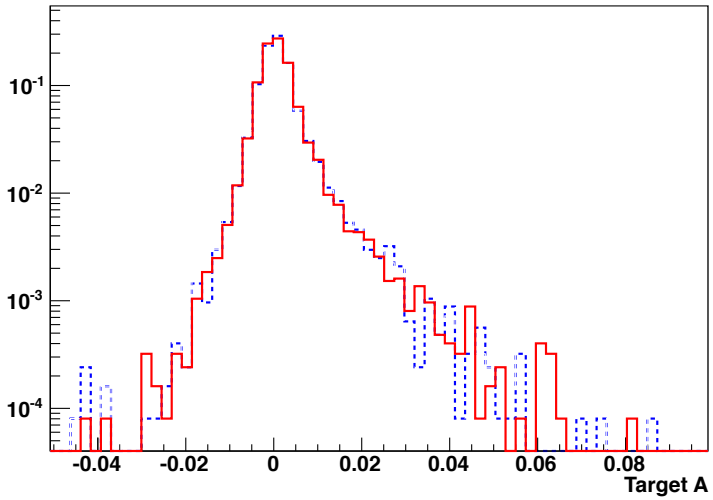
- K of them strongly correlated

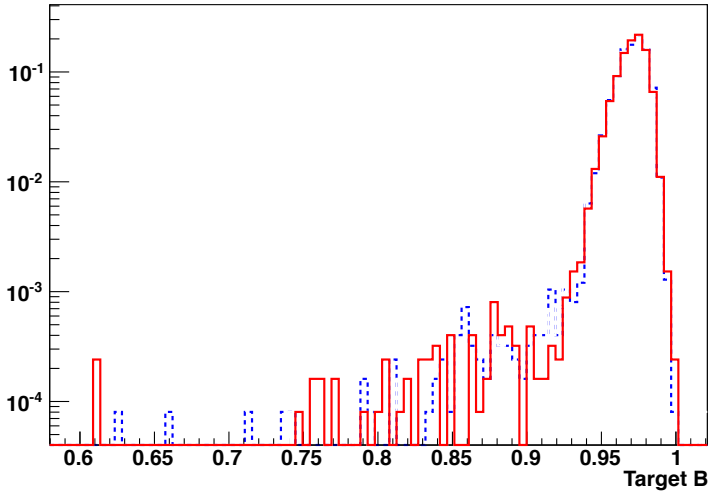
Y target outputs to estimate {A, B, C, D…}

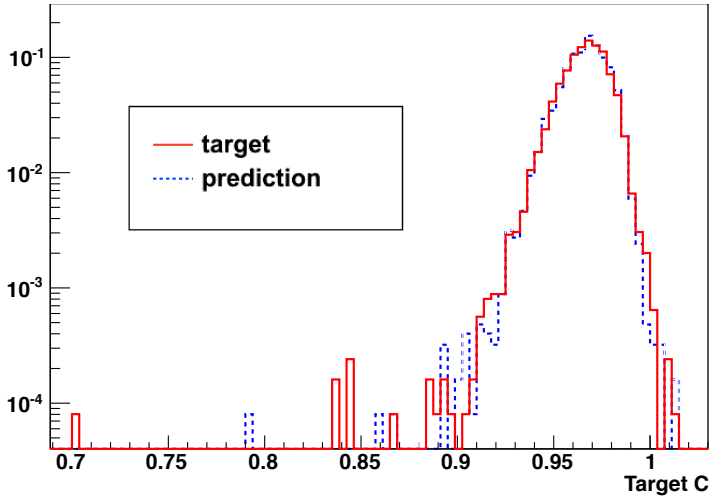
- N of them strongly correlated

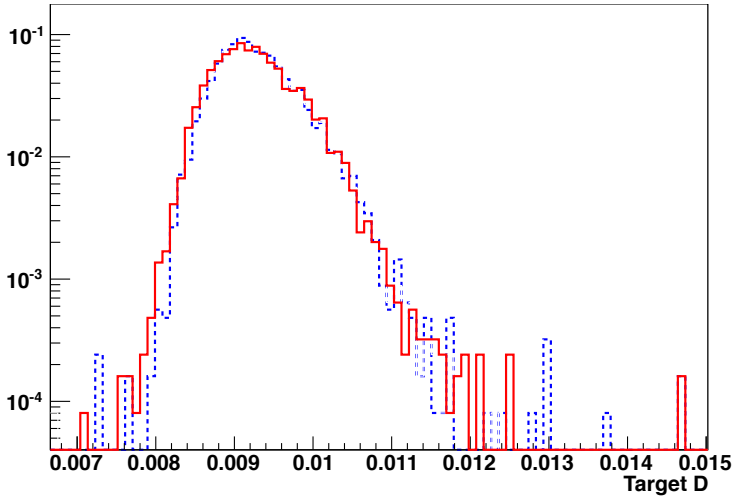
Challenge: build a predictive model to describe simultaneously all the outputs {A,B,C,D…}, provided a corresponding set of inputs.

Illustrative Example









Target Correlations

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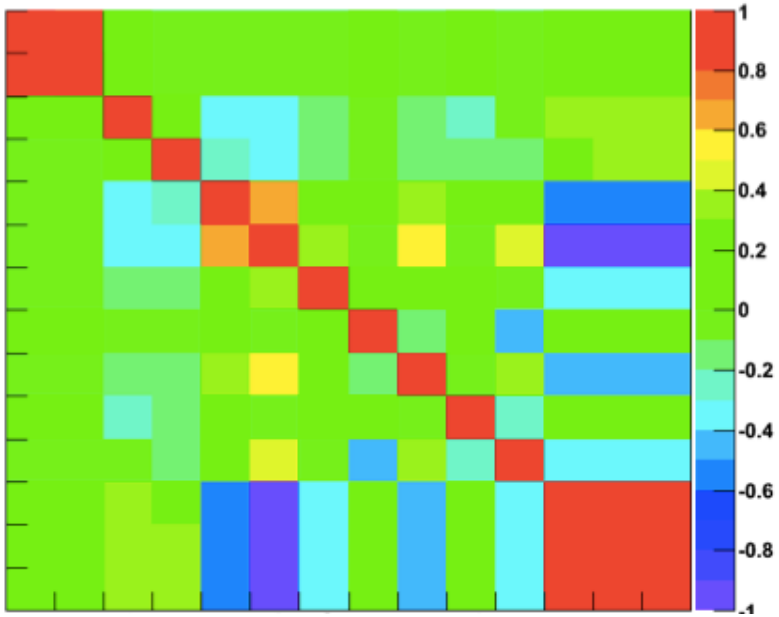
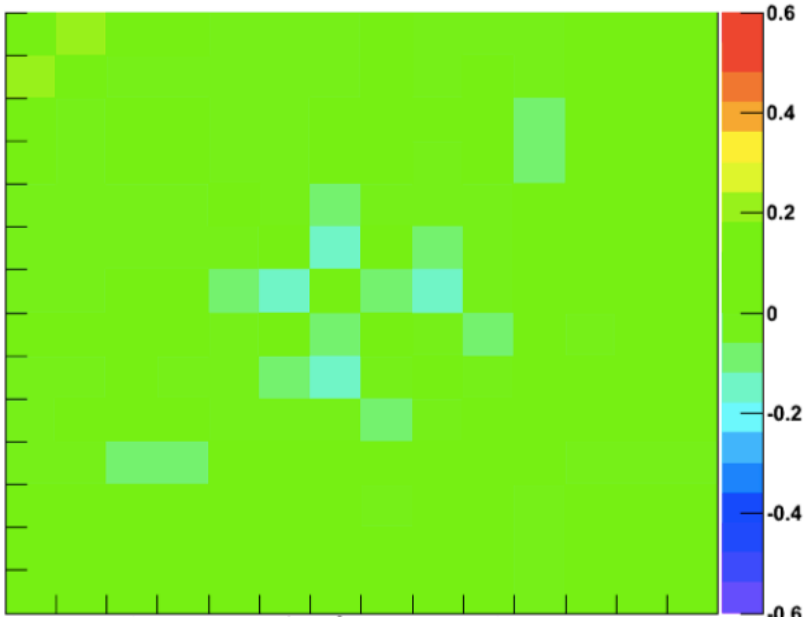


Prediction-Target Difference



Very close to Zero

Summary

- Multi-objective regression is a powerful tool
  - when you have multiple target functions to estimate simultaneously
  - better than N single-objective regressions especially when correlations need to be preserved
- Applications in HEP for learning multi-dimensional transformations or multi-parameter targets (for example in fast non-parametric simulation)