Interactive Machine Learning via Transparent Modeling: Putting Human Experts in the Driver’s Seat

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When is it Safe to Use Machine Learning in Healthcare?

- data for 1M patients
- 1000’s great clinical features
- train state-of-the-art machine learning model on data
- accuracy looks great on test set: AUC = 0.95

is it safe to deploy this model and use on real patients?
is high accuracy on test data enough to trust a model?
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is it safe to deploy this model and use on real patients?
NO! — human expert MUST be able to understand and edit model before use!
Motivation: Predicting Pneumonia Risk Study (mid-90’s)

- **LOW Risk**: outpatient: antibiotics, call if not feeling better
- **HIGH Risk**: admit to hospital (≈10% of pneumonia patients die)

One goal was to compare various ML methods:
- logistic regression
- rule-based learning
- k-nearest neighbor
- neural nets
- Bayesian methods
- hierarchical mixtures of experts
- ...

Most accurate ML method: **multitask neural nets**

Safe to use neural nets on patients?

- No — we used logistic regression instead...

Why???
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- RBL learned rule: $\text{HasAsthma}(x) \Rightarrow \text{LessRisk}(x)$

- True pattern in data:
  - asthmatics presenting with pneumonia considered very high risk
  - receive aggressive treatment and often admitted to ICU
  - history of asthma also means they often go to healthcare sooner
  - treatment lowers risk of death compared to general population

- If RBL learned asthma is good for you, NN probably did, too
  - if we use NN for admission decision, could hurt asthmatics

- Key to discovering $\text{HasAsthma}(x)$... was intelligibility of rules
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Lessons Learned

- Always going to be risky to use data for purposes it was not designed for
  - Most data has unexpected landmines
  - Not ethical to collect correct data for asthma

- Much too difficult to fully understand the data
  - Our approach is to make the learned models as intelligible as possible for task at hand

- Experts must be able to understand models in critical apps like healthcare
  - Otherwise models can hurt patients because of true patterns in data
  - If you don’t understand and fix model it will make bad mistakes

- Same story for race, gender, socioeconomic bias
  - The problem is in data and training signals, not learning algorithm

- Only solution is to put humans in the machine learning loop
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To put humans in the driver’s seat
all we need is an accurate, intelligible model
Problem: The Accuracy vs. Intelligibility Tradeoff

Intelligibility vs. Accuracy for different models:
- Boosted Trees
- Random Forests
- Neural Nets
- Single Decision Tree
- Logistic Regression
- Naive Bayes
- Decision Lists

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Intelligibility vs. Accuracy

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Model Space from Simple to Complex

- **Linear Model:** \( y = \beta_0 + \beta_1 x_1 + \ldots + \beta_n x_n \)

- **Additive Model:** \( y = f_1(x_1) + \ldots + f_n(x_n) \)

- **Additive Model with Interactions:** \( y = \sum_i f_i(x_i) + \sum_{ij} f_{ij}(x_i, x_j) + \sum_{ijk} f_{ijk}(x_i, x_j, x_k) + \ldots \)

- **Full Complexity Model:** \( y = f(x_1, \ldots, x_n) \)
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Generalized Additive Models (GAMs)
- Developed at Stanford by Hastie and Tibshirani in late 80’s
- Regression: $y = f_1(x_1) + ... + f_n(x_n)$
- Classification: $\text{logit}(y) = f_1(x_1) + ... + f_n(x_n)$
- Each feature is “shaped” by shape function $f_i$

T. Hastie and R. Tibshirani. 
*Generalized additive models.*
Skip technical details of algorithm and jump to results
Motivation: Predicting Pneumonia Risk Study (mid-90’s)

- Pneumonia Data (dataset from early 1990’s)
  - 14,199 pneumonia patients
  - 70:30 train:test split (train=9847; test=4352)
  - 46 features
  - predict POD (probability of death)
  - 10.86% of patients (1542) died
# Pneumonia Dataset (mid-90's): 46 Features

## Physical examination findings
- **Respiration rate (resps/min)**
  - ≤ 29*, ≥ 30
- **Heart rate (beats/min)**
  - ≤ 124*, 125–150, ≥ 151
- **Systolic blood pressure (mmHg)**
  - ≤ 60, 61–70, 71–80, 81–90, ≥ 91*
- **Temperature (°C)**
  - ≤ 34.4, 34.5–34.9, 35–35.5, 35.6–38.3*, 38.4–39.9, ≥ 40
- **Altered mental status (disorientation, lethargy, or coma)**
  - no*, yes
- **Wheezing**
  - no*, yes
- **Stridor**
  - no*, yes
- **Heart murmur**
  - no*, yes
- **Gastrointestinal bleeding**
  - no*, yes

## Laboratory findings
- **Sodium level (mEq/l)**
  - ≤ 124, 125–130, 131–149*, ≥ 150
- **Potassium level (mEq/l)**
  - ≤ 5.2*, ≥ 5.3
- **Creatinine level (mg/dl)**
  - ≤ 1.6*, 1.7–3.0, 3.1–9.9, ≥ 10.0
- **Glucose level (mg/dl)**
  - ≤ 249*, 250–299, 300–399, ≥ 400
- **BUN level (mg/dl)**
  - ≤ 29*, 30 to 49, ≥ 50
- **Liver function tests (coded only as normal* or abnormal)**
  - SGOT ≤ 63 and alkaline phosphatase ≤ 499*, SGOT > 63 or alkaline phosphatase > 499
- **Albumin level (gm/dl)**
  - ≤ 2.5, 2.6–3, ≥ 3.1*
- **Hematocrit**
  - 6–20, 20.1–24.9, 25–29, ≥ 30*
- **White blood cell count (1000 cells/µl)**
  - 0.1–3, 3.1–19.9*, ≥ 20
- **Percentage bands**
  - ≤ 10*, 11–20, 21–30, 31–50, ≥ 51
- **Blood pH**
  - 7.20, 7.21–7.35, 7.36–7.45*, ≥ 7.46
- **Blood pO₂ (mmHg)**
  - ≤ 59, 60–70, 71–75, ≥ 76*
- **Blood pCO₂ (mmHg)**
  - ≤ 44*, 45–55, 56–64, ≥ 65
What GA2Ms on Steroids Learn About Risk vs. Age
Splines tend to be too smooth
Some of the things the intelligible model learned:

- Age 105 is safer than Age 95
- We should have a retirement variable
  - Has_Asthma $\Rightarrow$ lower risk
  - History of chest pain $\Rightarrow$ lower risk
  - History of heart disease $\Rightarrow$ lower risk

Good we didn't deploy neural net back in 1995

But can understand, edit and safely deploy intelligible GA2M model

Intelligible/transparent model is like having a magic pair of glasses

Model correctness depends on how model will be used
  - this is a good model for health insurance providers
  - but needs to be repaired to use for hospital admissions

Important: Must keep potentially offending features in model!
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Parity is the classic (extreme) interaction
- For N-bit parity, need all N bits at the same time to calculate parity
- No correlation between any of the bits and parity signal
- No information in any subset of the bits

Interactions can’t be modeled as sum of independent effects

Interactions important on some problems, less on others
Work in Progress: Can We Make GA2Ms More Intelligible?

- Over-Parameterization
- Smoothness
- Sparsity
- Monotonicity
- Lasso L1 Regularization (feature selection)
- Tradeoff between simplicity/intelligibility and prediction accuracy
- More causal?
- ...
Over-Paramterization

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GA2Ms with pairwise interactions are over-parameterized

What is over-parameterization?

- suppose $y = a \times x_1 + b \times x_1$
- many ways to set $a$ and $b$ to yield same model because $y = (a + b) \times x_1$
- suppose we want $y = 10 \times x_1$
- then $a = 10$ and $b = 0$, or $a = 5$ and $b = 5$, or even $a = 100$ and $b = -90$ all work

There’s a similar over-parameterization between mains and interactions of those mains
Over-Parameterization: After Moving All Mass From Main to Interaction

![Graphs showing the relationship between age and pneumonia risk score](image1.png)

![Heatmap showing the relationship between cancer and age](image2.png)
Over-Parameterization: After Moving All Mass From Main to Interaction

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IDEA2017: Transparent ML

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Work in Progress: Can We Make GA2Ms More Intelligible?

- Over-Paramterization
  - Pushing all mass into interactions can reduce number of terms because some mains go away
  - But can make model harder to interpret because interactions can become more complex
  - If main is involved in more than one interaction, many ways to distribute mass
  - GA2M algorithm currently tries to push mass into mains so pairs are just residuals
  - But over-parameterization and mass-moving provide interesting interactive opportunities

- Smoothness

- Sparsity

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- **Smoothness**
- **Sparsity**
- **Monotonicity**
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- **Tradeoff between simplicity/intelligibility and prediction accuracy**
- **More causal?**
- **...**
Smoothness: Before and After Optimizing Smoothness of Main Effect

![Graphs showing smoothness comparison](image)
Smoothness: Before and After Optimizing Smoothness of Main Effect

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IDEA2017: Transparent ML
August 16, 2017
Over-Paramterization

Smoothness
- to add constraint like smoothness to main must add counter-balancing constraint to interactions otherwise optimization will happily move all mass from main to interaction!
- can achieve simpler, cleaner main but at expense of pushing detail into interactions
- in general, we don’t find extreme smoothness of mains is to be preferred
- smoothness created monotonicity (by accident), making it look like \( \text{age} > 100 \) is solved
- but adding explicit constraint for monotonicity is a better way to achieve monotonicity

Sparsity

Monotonicity

Lasso L1 Regularization (feature selection)

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- More causal?
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Sparsity: Before and After Optimizing Sparsity of Interactions

![Graph showing sparsity changes]

![Heatmap comparing ages and cancer stages]
Sparsity: Before and After Optimizing Sparsity of Interactions

![Graph 1: Age vs. Pneumonia Risk Score](image1)

![Graph 2: Age vs. Mean-Centered Pneumonia Risk Score](image2)

![Heatmap 1: Age vs. Cancer](image3)

![Heatmap 2: Age vs. Cancer](image4)
Work in Progress: Can We Make GA2Ms More Intelligible?

- Over-Parameterization
- Smoothness
- Sparsity
  - Don’t have to add counter-balance because can’t move all of an interaction to the mains
  - Adding sparsity (or smoothness) to interactions can make them easier to interpret
  - Sometimes seems to hurt mains a little, sometimes doesn’t
- Monotonicity
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Lasso L1 Regularization (feature selection)

Tradeoff between simplicity/intelligibility and prediction accuracy

More causal?

...
Smoothness + Sparsity + Monotonicity + Simplicity + L1 + ...

- Most machine learning is about optimizing well-defined criteria such as accuracy

- For each term in a GA2M model (can be 100’s or 1000’s of terms)
- For each main M and pairwise interaction PI in a GA2M model
- Have the opportunity to optimize smoothness, sparsity, monotonicity, simplicity, L1, ...
- To optimize things like intelligibility, editability, trust, ...

- Don’t have objective measures for these so we can’t do optimization automatically

- Currently need interactive exploration by human to examine the possibilities
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Work in Progress: Can We Make GA2Ms Easier to Edit?

- Centering to increase modularity
- HCI tools to help experts edit model and understand the impact of those edits
- Statistical tools to help experts understand the impact of their edits on accuracy
Centering to increase modularity

HCI tools to help experts edit model and understand the impact of those edits

Statistical tools to help experts understand the impact of their edits on accuracy
Modularity of terms makes GA2Ms easier to edit — can we improve modularity?
Yes, one easy fix: add intercept term to make each term easier to remove

Suppose $y = mx + b$
Can’t change $m$ or $b$ without changing model

Now suppose $y = m \ast \text{graph}(x) + b$
Can shift graph up or down, and just compensate by adjusting $b$
$y = m \ast (\text{graph}(x) + c) + b’$ where $b’ = b – m \ast c$

This is useful for GA2Ms because removing a term (graph) introduces bias
By centering each graph so mean prediction is zero, we make graphs removable
Work in Progress: Can We Make GA2Ms Easier to Edit: Centering

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Can’t change \( m \) or \( b \) without changing model

Now suppose \( y = m \ast graph(x) + b \)
Can shift graph up or down, and just compensate by adjusting \( b \)
\( y = m \ast (graph(x) + c) + b' \) where \( b' = b - m \ast c \)

This is useful for GA2Ms because removing a term (graph) introduces bias
By centering each graph so mean prediction is zero, we make graphs removable
Work in Progress: Can We Make GA2Ms Easier to Edit: Analysis Tools

- What is the impact of editing model on overall accuracy?
- What is the impact to different kinds of patients?
  - Could edit(s) be accomplished just by pushing mass around?
  - NO! — this is cheating, using mass moving to hide/shuffle mass!
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- It is much easier to understand a model than to understand the data
- The model will tell you things about the data you never expected
- Don’t have to know what to look for in advance
- Don’t have to design statistical tests for biases in advance
- Just train model, and look at what it learned — the model will surprise you

- Modularity of GAMs makes many problems easier to recognize
- Modularity of GAMs makes many problems easier to correct

- High accuracy of GA2Ms means less is missing — GA2M model often is as accurate as any other model black-box we could train on data
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GA2Ms are intelligible only if features are intelligible.

GA2Ms are not a replacement for deep learning on raw signals. Does not work as well as deep nets on pixels, speech signals, … works best on features crafted by humans.

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High accuracy on test set is not enough
There are land mines hidden in the data
You need magic glasses to see the landmines
It’s critical to understand model before deploying it
Model correctness depends on how model will be used
New GA2Ms give us accuracy and intelligibility at same time
Important to keep potentially offending variables in model so bias can be detected and then removed after training
If you eliminate offending variables before training you:
  can't tell you have a problem
  make it harder to correct the problem
Transparency allows you to detect problems you didn’t anticipate in advance
Working to develop tools to put expert in the driver’s seat — need your help!
Intelligible Models or Black Box?

Rich Caruana (Microsoft Research)
30-day Hospital Readmission Data

- larger, modern dataset
- records from NYP 2011-2014
- train=195,901 (2011-12); test=100,823 (2013)
- 3,956 features for each patient
- goal: predict probability patient will be readmitted within 30 days
- 8.91% of patients readmitted within 30 days
Quick look at two 30-day Readmission Patients
References

Y. Lou, R. Caruana, and J. Gehrke.  
*Intelligible Models for Classification and Regression.*  
In *KDD*, 2012.

*Accurate Intelligible Models With Pairwise Interactions.*  
In *KDD*, 2013.

*Intelligible Models for Healthcare.*  
In *KDD*, 2015.

T. Hastie and R. Tibshirani.  
*Generalized additive models.*  
Thank You!
GA^2M Algorithm Sketch

- **Stage 1**: build best additive model using only 1-dim components
  - Additive effects are now modeled
  - If Stage 1 done perfectly, only have interaction (and noise) in residuals

- **Stage 2**: fix the one-dimensional functions
  - Detect pairwise interactions on residuals (new FAST algorithm)

- **Stage 3**: build shape models for most important pairwise interactions on residuals

- **Stage 4**: post-process shape plots
  - center average prediction of each plot to improve modularity
  - sort terms by importance to aid intelligibility

- Bag (repeat) process 10-100 times to create pseudo-confidence intervals and further reduce overfitting