Unleashing Modern AI in Pharmaceutical and Chemical Industries

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AI Suitcase

- **Reactive Machines:**
  - These are basic rule-based systems that operate based on predefined rules.
- **Expert Systems:**
  - These are computer systems that mimic the decision-making ability of a human expert in a specific domain.
- **Machine Learning (ML) Systems:**
  - ML is a subset of AI that focuses on developing algorithms and models that enable computers to learn from data.
  - Types of ML systems include **supervised learning (PA)**, unsupervised learning, and reinforcement learning.
- **Neural Networks:**
  - Inspired by the human brain, neural networks are a key component of many AI systems.
- **Narrow/Generative LLM AI (Weak AI):**
  - These AI systems are designed and trained for a specific task or a narrow set of tasks.
  - Examples include virtual personal assistants, image recognition software, and language translation services.
- **Limited Memory:**
  - These AI systems can learn from historical data to make better decisions.
  - Self-driving cars often use limited memory AI to navigate based on past experiences.
  - Can be integrated into robots to enable them to learn and interact with the environment.
- **Self-aware AI:**
  - This refers to hypothetical AI systems with self-awareness and consciousness.
- **Theory of Mind:**
  - This is a more advanced form of AI that can understand human emotions, beliefs, intentions, and thoughts.
- **General AI (Strong AI):**
  - General AI systems can understand, learn, and apply knowledge across diverse domains.
  - They can perform any intellectual task that a human being can do.
- **Superintelligent AI:**
  - This is a theoretical AI that surpasses human intelligence in every aspect.

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Text In Text Out

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AGI / Science Fiction / Religion

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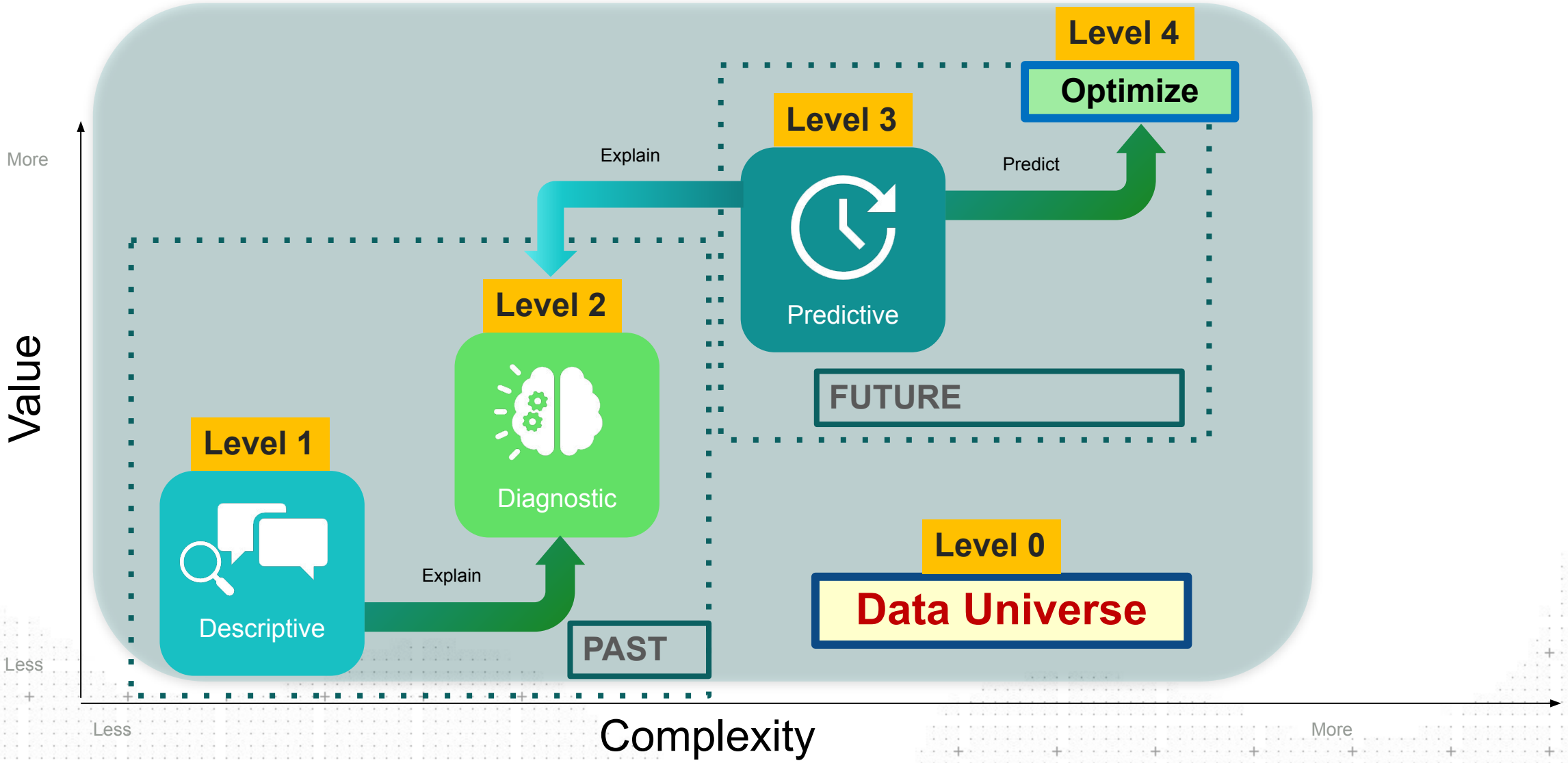
Levels of Data Analytics



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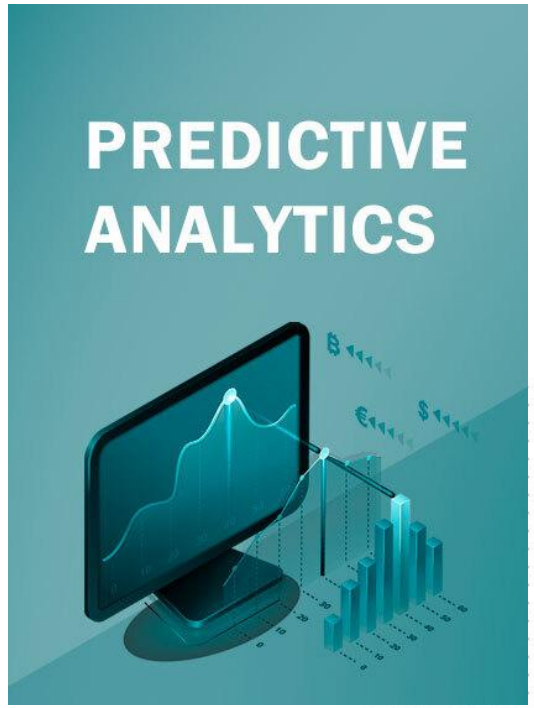
Predictive AI: The Essence and Utility

- **Predict** [something] **based on** [something else]
- **Direct Application (Level 3)**: use a PA model to predict the outcome of interest
  - Emphasis on the **accuracy** of predictions
- Link to **Diagnostic Analytics (Level 2)**: use a PA model to explain why such and such predictions are made
  - Emphasis on the **explanation** of predictions
- Link to **Response Optimization (Level 4)**: use a PA model to discover optimal inputs to achieve a desired outcome
  - Emphasis on the **discovery** of the optimal inputs
- **Key tradeoff**: simple and easy to explain models tend to be less accurate!



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Traditional Predictive AI (a.k.a. Machine Learning)

Numbers In
Numbers Out

- To engage in conventional predictive AI, we **must have**:
- **Clear Problem Definition** – **predict** something **based on** something else
- **Historical Dataset** – a fixed grid of **observations** by **variables**
- **Response/Target variable** – what we want to predict (**all sides** must be captured by the historical data)
  - **Regression Problem** – the target variable is **continuous** (Energy, Score, etc.)
  - **Classification Problem** – the target variable is **categorical** (Region, Color, etc.)
- **Predictor variables** – variables used to predict the response (any combination of continuous and categorical variables)

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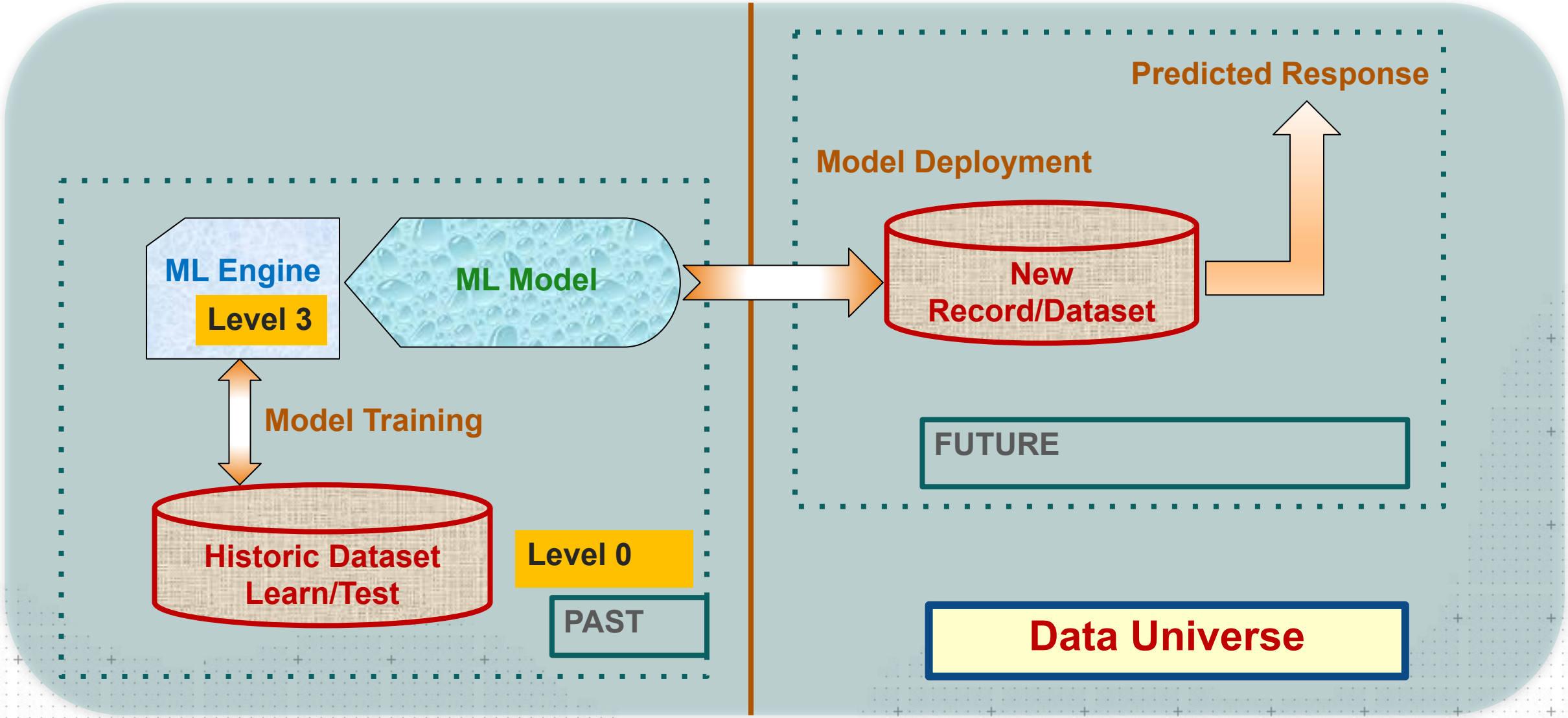
Machine Learning Process



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Classical vs Modern Approaches in ML

- **Classical approach**: I will dictate what the model structure is, the data will be used to fit in the details
  - Multiple linear regression
  - Logistic regression
  - PLS, Lasso, etc.

Dictate to the data

Easy to explain
Easy to fail
Compute Light

- **Modern approach**: I will let the data tell me what the model is
  - **CART** – **C**lassification **A**nd **R**egression **T**rees
  - **MARS** – **M**ultivariate **A**daptive **R**egression **S**plines
  - **RF** – **R**andom **F**orest
  - **TN** – **T**ree **N**et (a.k.a. Stochastic Gradient Boosting)

Learn from the data

Hard to explain
Hard to fail
Compute Intense

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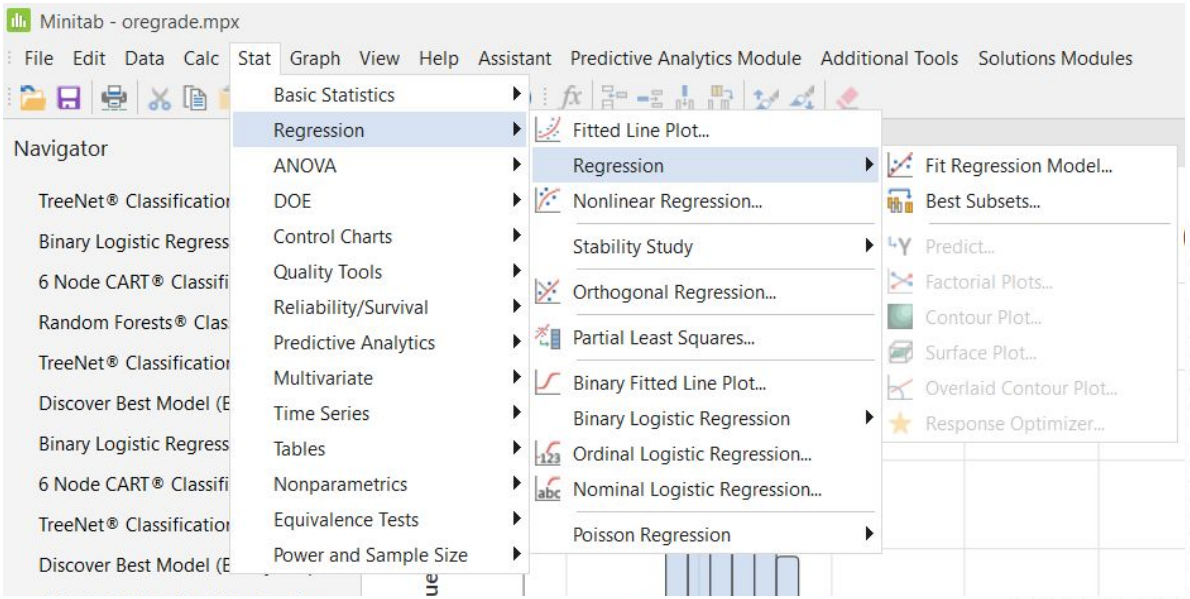
Classical Algorithms: Common Features

- **Parametric** in nature (well-defined equations)
- Based on certain statistical/distributional **assumptions**
- **Assume expert knowledge of the problem**
- The model shape (response surface) is **dictated** by the analyst
- All observations contribute **globally**
- Focus solely on reducing the **variance** of estimates
- Give **baseline accuracy**
- Work great on **small** datasets



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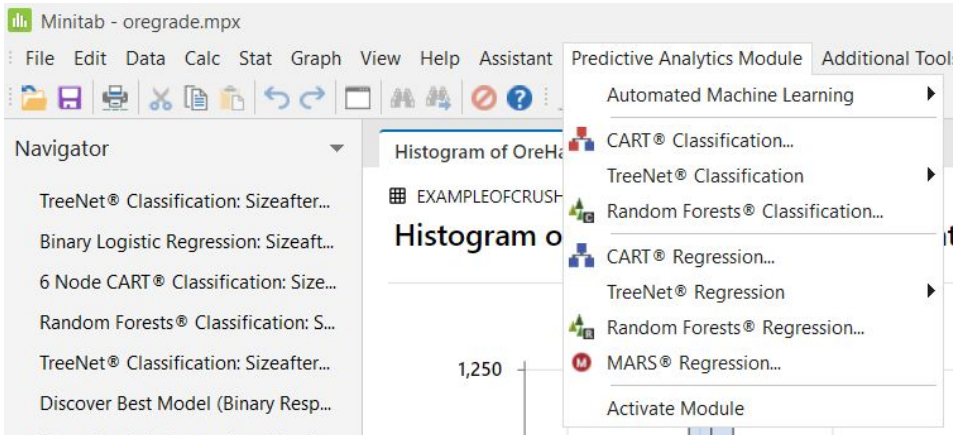
Modern Algorithms: Common Features

- **Non-parametric** in nature (no equations)
- **Do not rely** on statistical/distributional assumptions
- **Learn from the data**
- The model shape (response surface) is **developed dynamically** by scrutinizing the data
- Observations contribute **locally**
- Focus on the **bias/variance tradeoff** by giving a **range** of models
- Give **superior accuracy**
- Work great on **medium to large** datasets



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Uses of Modern ML in Pharma and Chemical Industries

- Drug Discovery and Development
  - **QSAR** (Quantitative Structure-Activity Relationship) Modeling based on molecular descriptors and fingerprints
  - **Virtual Screening** (Hit Discovery) – to filter large compound libraries to identify potential candidates
  - **ADMET Predictions** (Absorption, Distribution, Metabolism, Excretion, Toxicity)
- Chemical Manufacturing and Process Optimization
  - Process Control and Yield Prediction
  - Fault Detection and Root Cause Analysis
- Clinical Research and Personalized Medicine
  - Ranking genomic, proteomic, or metabolomic features associated with treatment response
  - Clinical trial optimization – predicting patient dropout, adverse effects, treatment response
- Toxicology and Environmental Risk Assessment
- Pharmaceutical Formulation, Polymer and Material Design

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Published Uses of ML in Recent Research

Industry/Application	Method	Highlights & Outcomes
Pharmaceutical shipping optimization	LightGBM (GBM)	96% accuracy in mode selection SpringerLink +1
Chemical functional use prediction (QSUR)	Random Forest	Screened ~6,400 chemicals; strong performance actiac.org
Sulphonation product quality modeling	Random Forest	MAE 0.089, corr. 0.978 arXiv
Soft-sensing (detergent quality)	Random Forest	Top 3 features achieved strong prediction arXiv
Iron oxide synthesis (phase & size control)	Random Forest	96% phase, 81% size accuracy; parameter recommendations arXiv
Zinc filtration moisture modeling	Random Forest	Outperformed SVR in predictive accuracy arXiv

Case Study 1: Personalized Medicine

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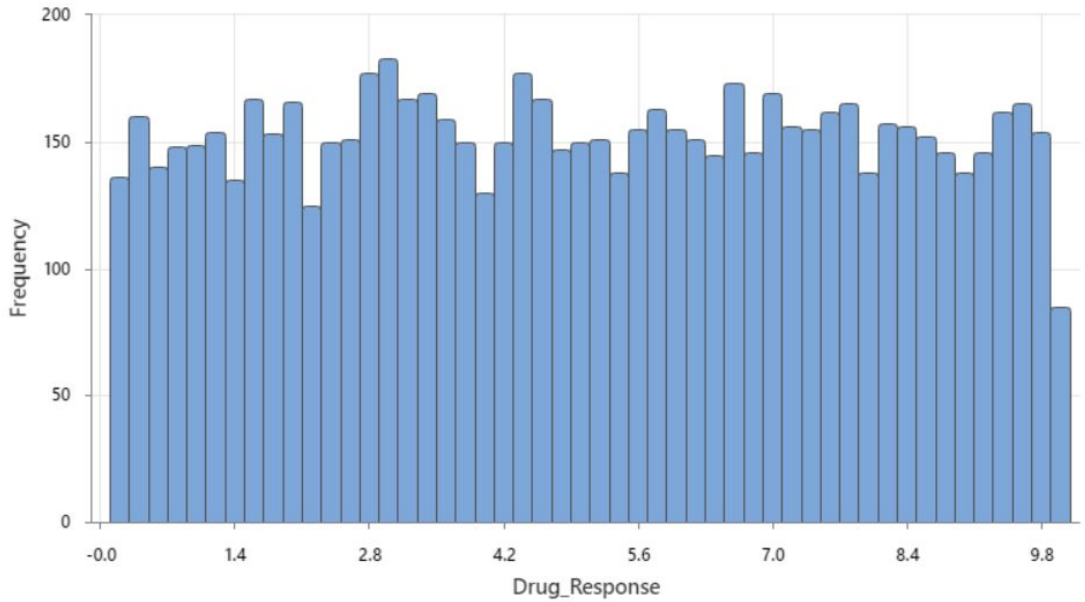
Personalized Medicine Research

C70	C71	C72-T	C73-T	C74-T	C75-T	C76-T	C77
Protein_Score_9	Protein_Score_10	Pathway_1	Pathway_2	Pathway_3	Pathway_4	Pathway_5	Drug_Response
0.194099	0.589134	Low	High	Moderate	Moderate	Low	9.44071
0.391995	0.223219	Low	Low	High	High	Low	8.91781
0.952073	0.440213	High	Low	High	Low	Low	9.06261
0.867519	0.323174	Moderate	Moderate	High	Low	High	9.03005
0.669718	0.769588	Low	Low	High	Moderate	High	8.75017
0.180836	0.519773	High	Low	Low	High	High	7.13843
0.779635	0.725349	Moderate	High	Low	Low	Moderate	0.93278



- A dataset containing 7643 patient profiles
  - 50 key gene expressions
  - 10 mutation indicators
  - 10 protein scores
  - 5 pathways (low, moderate, high)
- Want to predict continuous drug response
- This is a regression problem with 60 continuous and 15 categorical predictors

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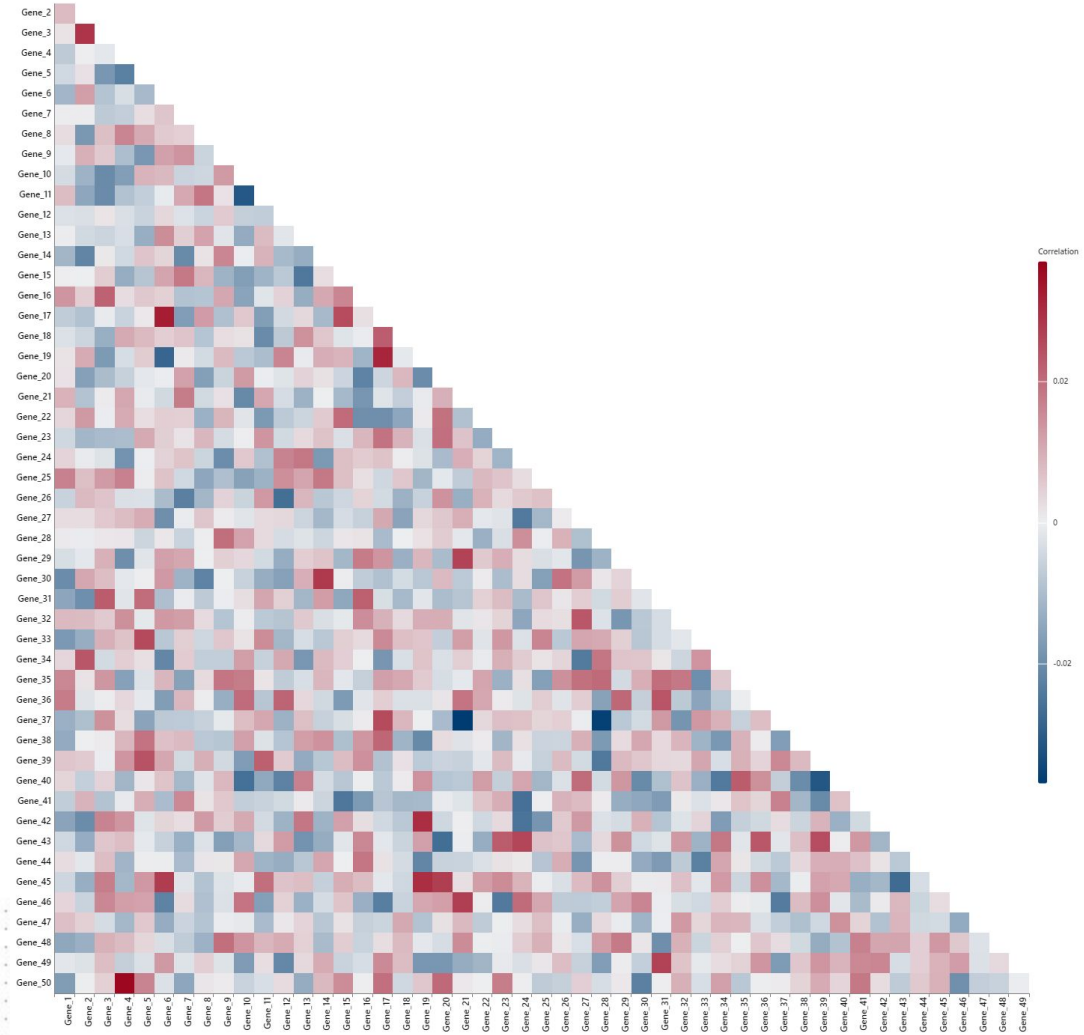
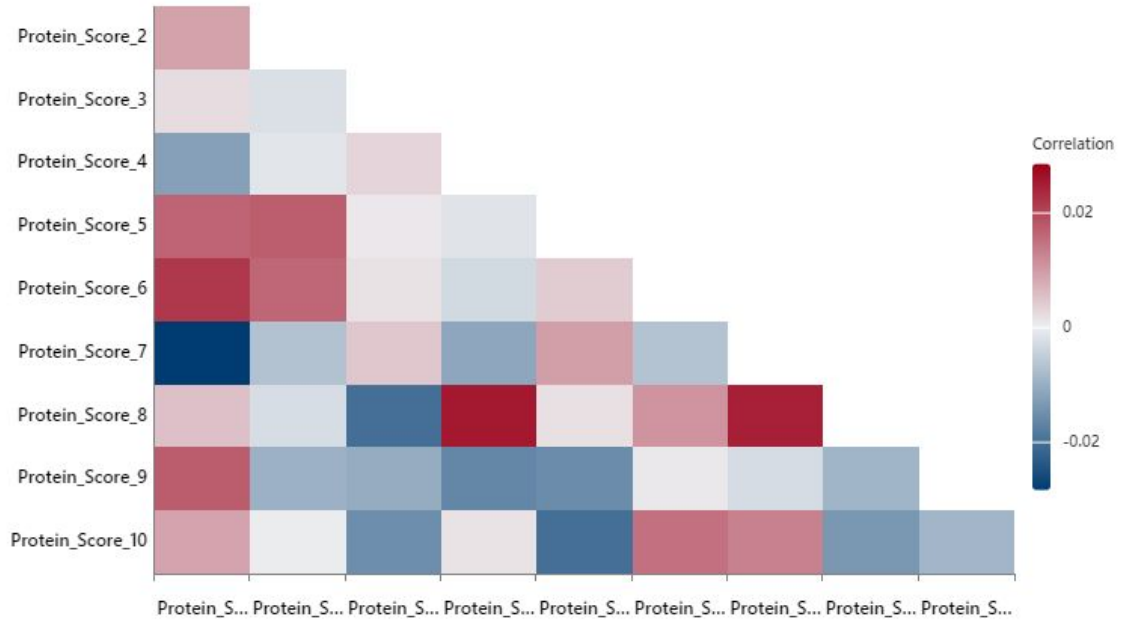
Level 1: Descriptive





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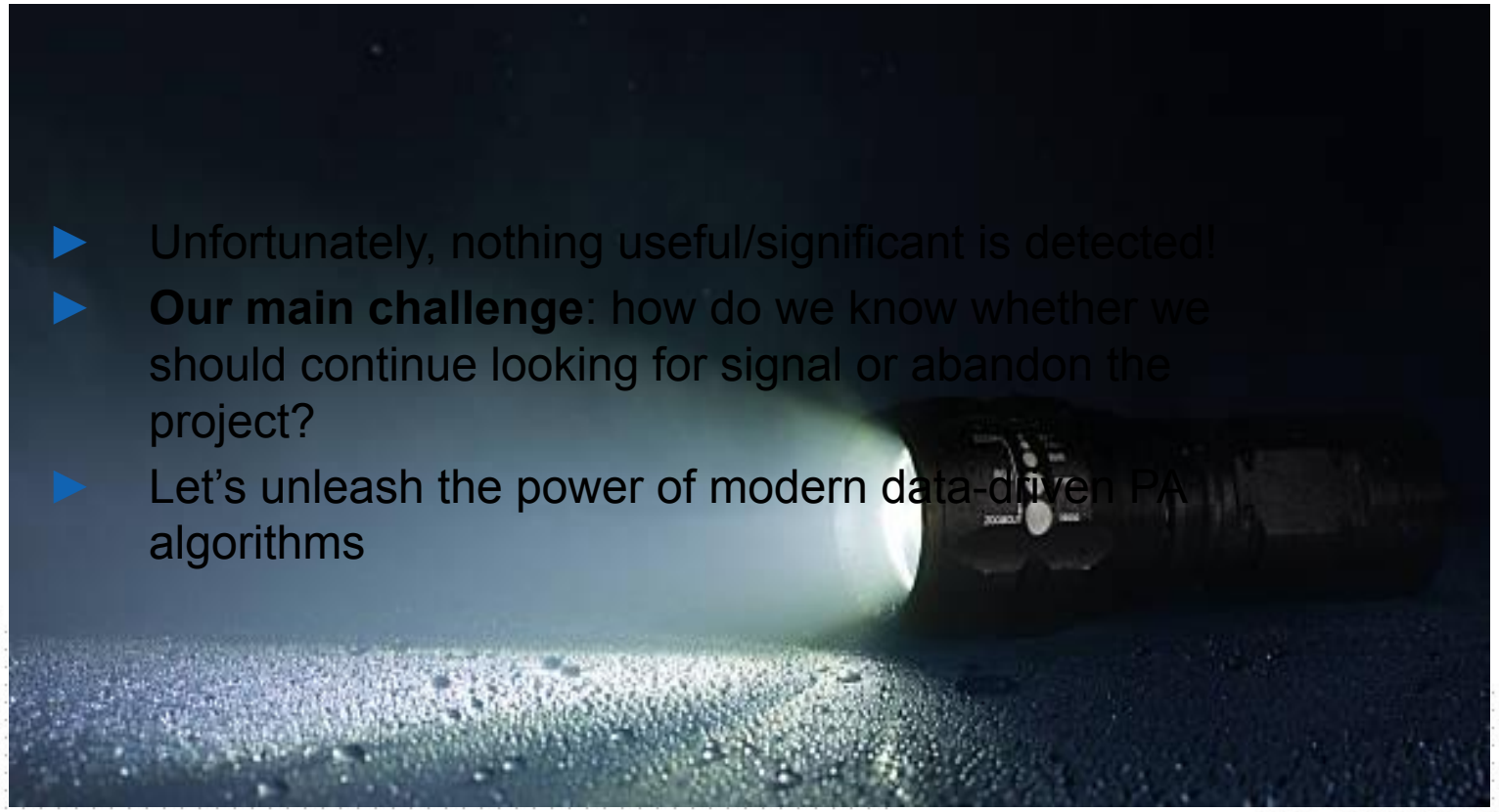
Conventional Regression Model

Model Summary

S	R-sq	R-sq(adj)	R-sq(pred)	Test S	Test R-sq
2.84268	1.31%	0.97%	0.61%	2.82412	0.00%



- Unfortunately, nothing useful/significant is detected!
- **Our main challenge**: how do we know whether we should continue looking for signal or abandon the project?
- Let's unleash the power of modern data-driven PA algorithms

Coefficients

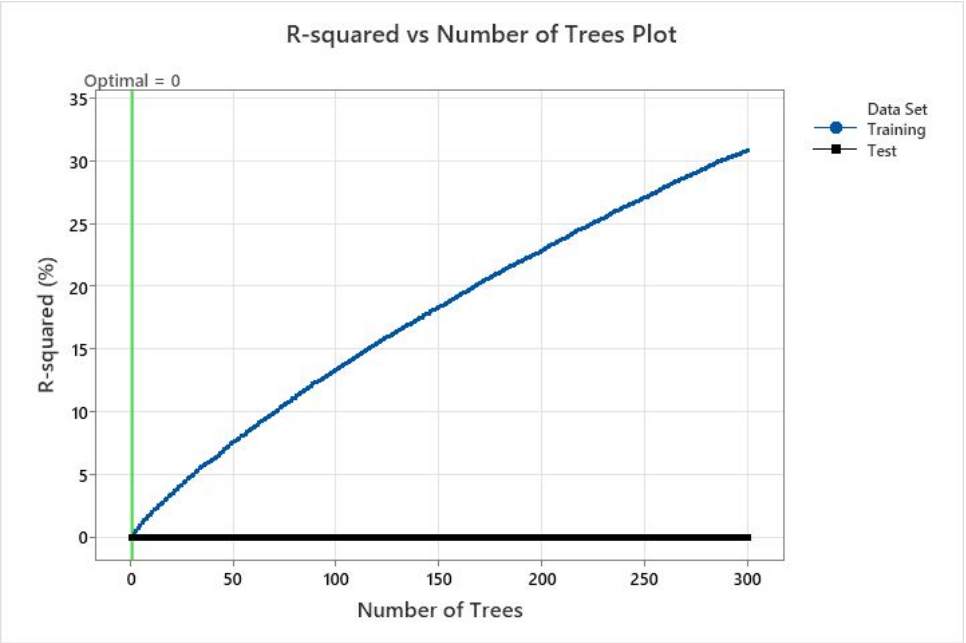
Term	Coef	SE Coef	T-Value	P-Value	VIF
Constant	6.081	0.267	22.81	0.000	
Gene_1	0.0272	0.0134	2.03	0.042	1.00
Gene_9	-0.0231	0.0135	-1.71	0.087	1.00
Gene_11	-0.0215	0.0135	-1.60	0.110	1.00
Gene_15	-0.0318	0.0135	-2.35	0.019	1.00
Gene_17	-0.0199	0.0136	-1.46	0.144	1.00
Gene_23	-0.0302	0.0135	-2.23	0.026	1.00
Gene_26	-0.0233	0.0134	-1.74	0.082	1.00
Gene_29	-0.0248	0.0134	-1.85	0.065	1.00
Gene_31	-0.0259	0.0135	-1.92	0.054	1.00
Gene_35	0.0217	0.0135	1.61	0.107	1.00
Gene_39	-0.0328	0.0133	-2.46	0.014	1.00
Gene_41	-0.0293	0.0134	-2.18	0.029	1.01
Protein_Score_1	0.328	0.136	2.41	0.016	1.00
Protein_Score_10	-0.324	0.136	-2.38	0.017	1.00
Mutation_3					
1	0.1347	0.0779	1.73	0.084	1.00
Mutation_6					
1	-0.1779	0.0778	-2.29	0.022	1.00
Pathway_2					
Low	0.2110	0.0953	2.21	0.027	1.34
Moderate	0.0498	0.0955	0.52	0.602	1.34

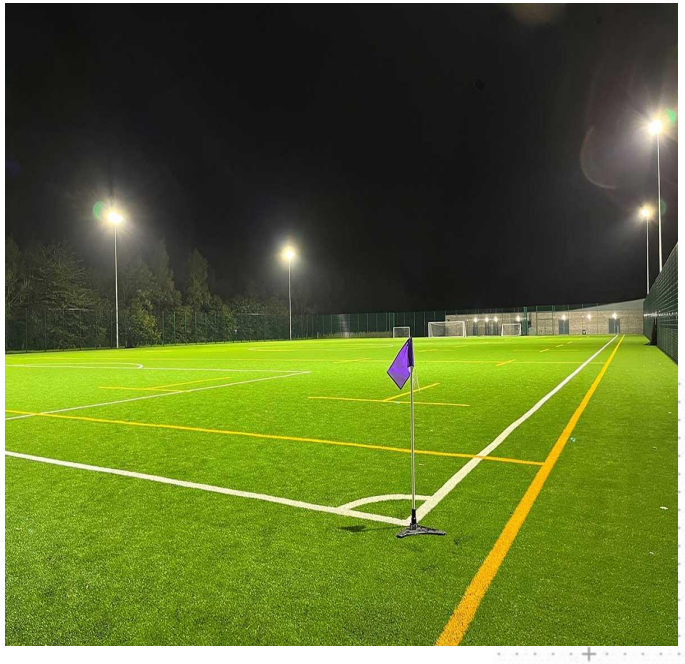
Modern PA Model (TreeNet)

Model Summary

Total predictors	75
Important predictors	5
Number of trees grown	300
Optimal number of trees	1

Statistics	Training	Test
R-squared	0.13%	0.00%
Root mean squared error (RMSE)	2.8347	2.8520
Mean squared error (MSE)	8.0354	8.1340
Mean absolute deviation (MAD)	2.4571	2.4669
Mean absolute percent error (MAPE)	1.6172	1.5236





- We have a **final confirmation**: there is no empirical evidence to support our initial hypothesis that the drug response can be different depending on the genomic and proteomic profile of the patient
- Further research might focus on **finding different genes and proteins** by collecting more data

Case Study 2: Virtual Screening Using Molecular Fingerprints

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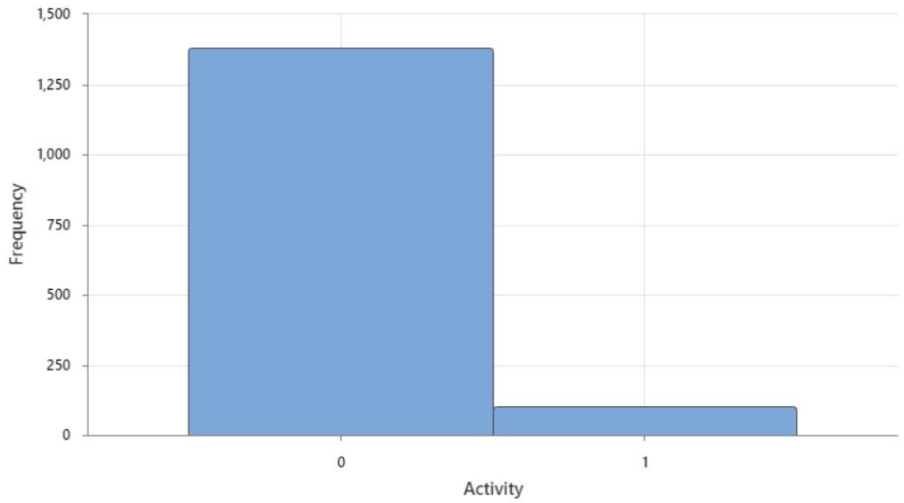
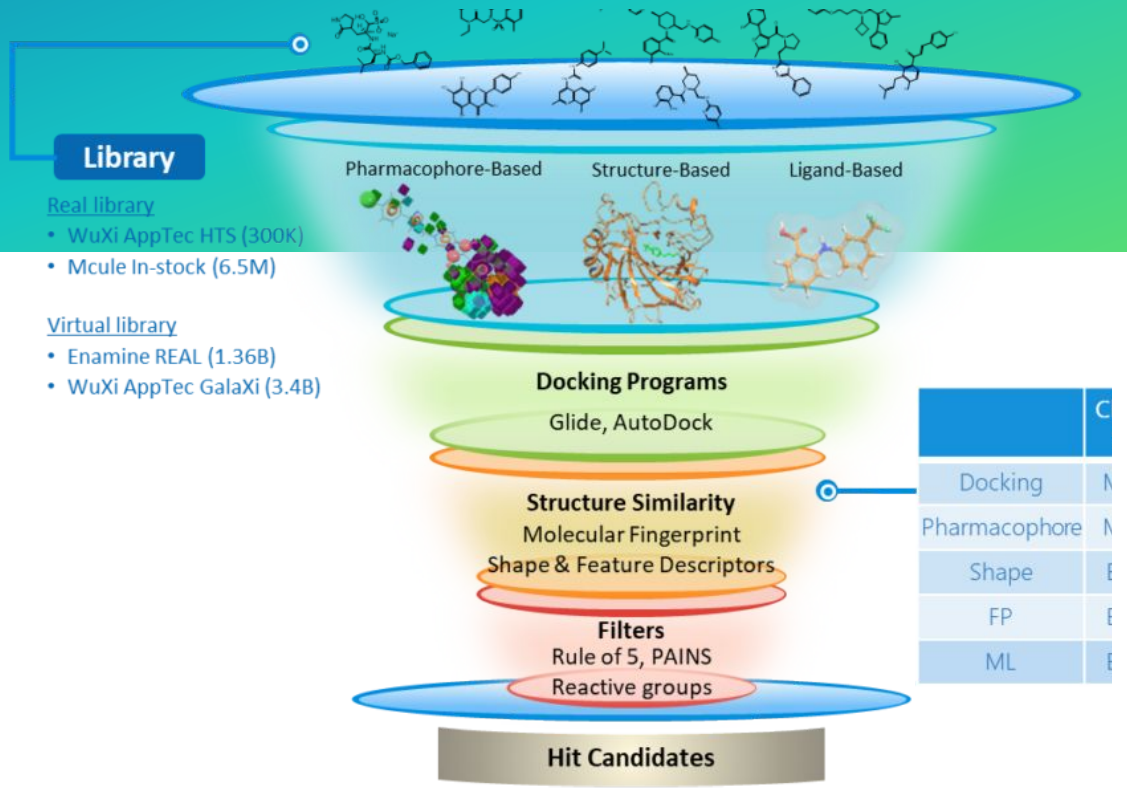
Virtual Screening Dataset

C1020	C1021	C1022	C1023	C1024	C1025
1019	1020	1021	1022	1023	Activity
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	1
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0





- A dataset containing 1484 binary fingerprints of different compounds
  - 1024 indicators for each fingerprint
- Want to predict binary activity response for further screening
- This is a binary classification problem with 1024 binary predictors

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Conventional Logistic Regression Model

Binary Logistic Regression: Activity versus 0, 1, 2, 3, 4, 5, 6, 7, 8, 9,

* ERROR * The training data set must contain all levels of the categorical predictors.

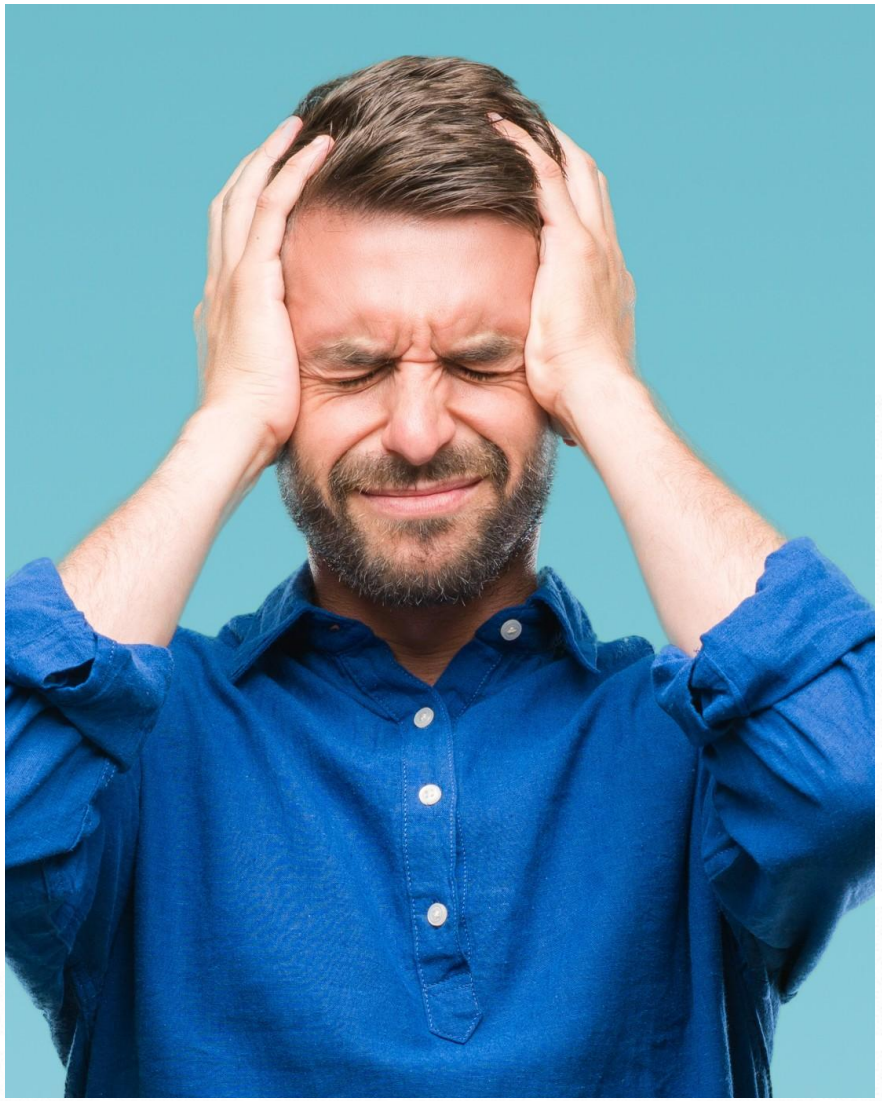
Binary Logistic Regression: Activity versus 0, 1, 2, 3, 4, 5, 6,

* ERROR * Continuous predictors must have more than one distinct value.

Binary Logistic Regression: Activity versus 0, 1, 2, 3, 4, 5, 6,

* ERROR * Categorical predictors must have more than one distinct value.

- Unfortunately, we struggle with the **data requirements!**
- **Solution**: Unleash modern PA on it!



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Modern PA Model: TreeNet

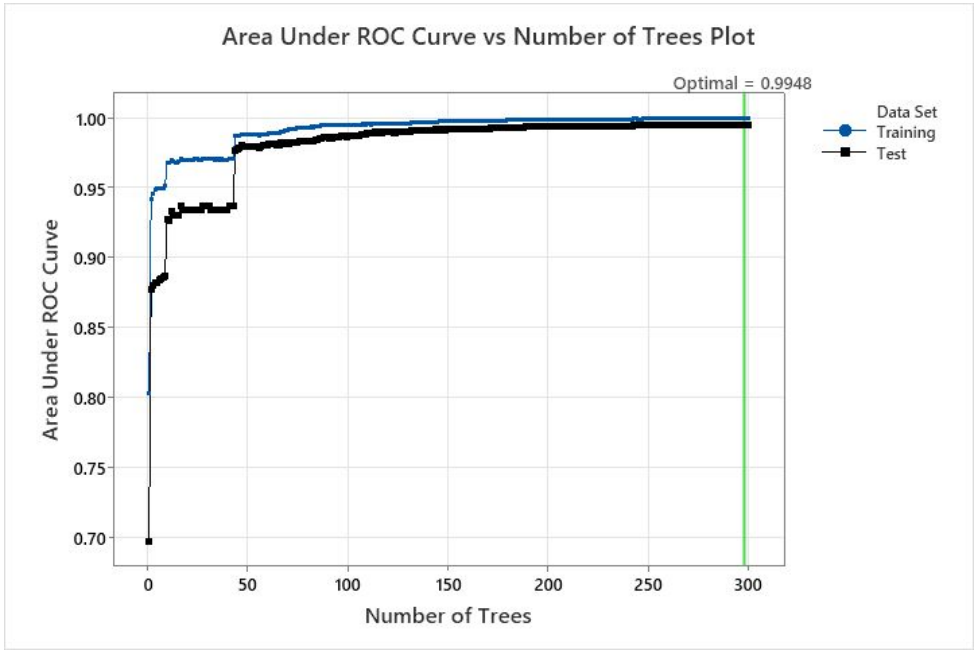
Binary Response Information

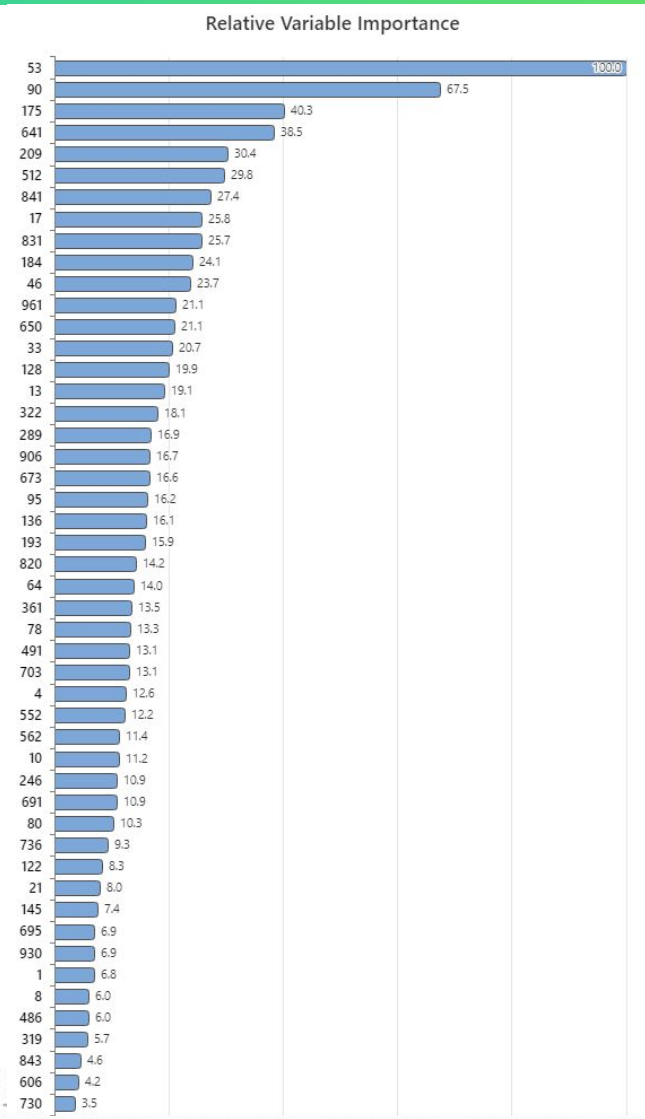
Variable	Class	Training Count	Training %	Test Count	Test %
Activity	1 (Event)	74	7.07	30	6.86
	0	973	92.93	407	93.14
	All	1047	100.00	437	100.00

Model Summary

Total predictors	1024
Important predictors	58
Number of trees grown	300
Optimal number of trees	298

Statistics	Training	Test
Average -loglikelihood	0.0393	0.0553
Area under ROC curve	0.9995	0.9948
95% CI	(0.9988, 1)	(0.9884, 1)
Lift	10.0000	9.3333
Misclassification rate	0.0086	0.0137





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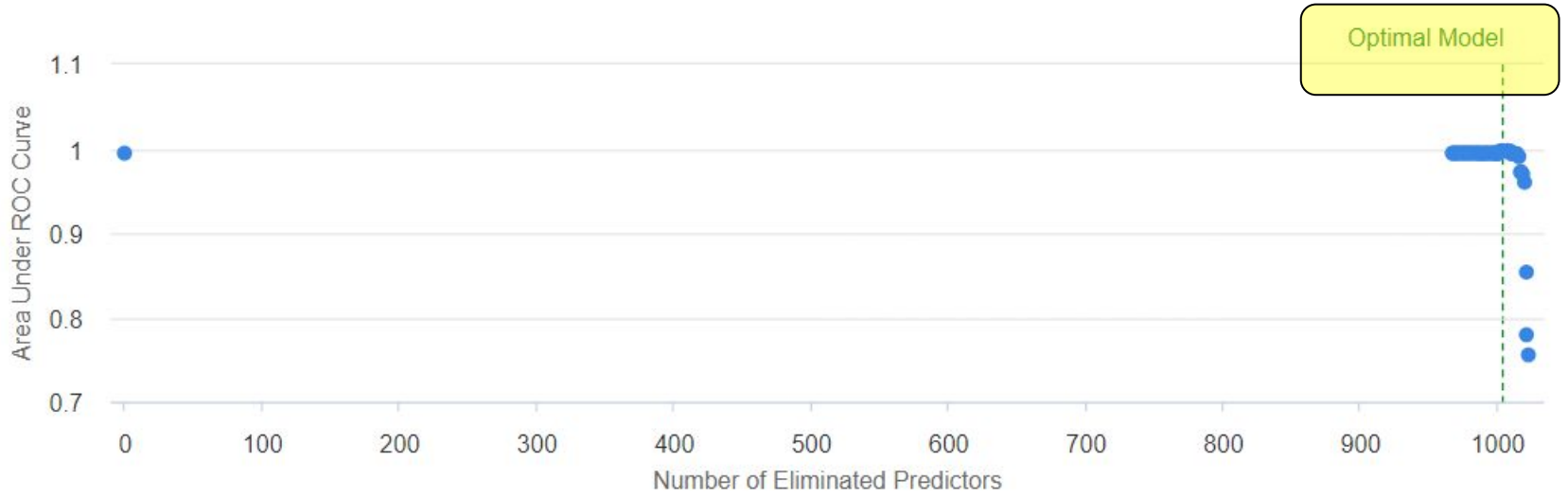
Predictor Discovery AI



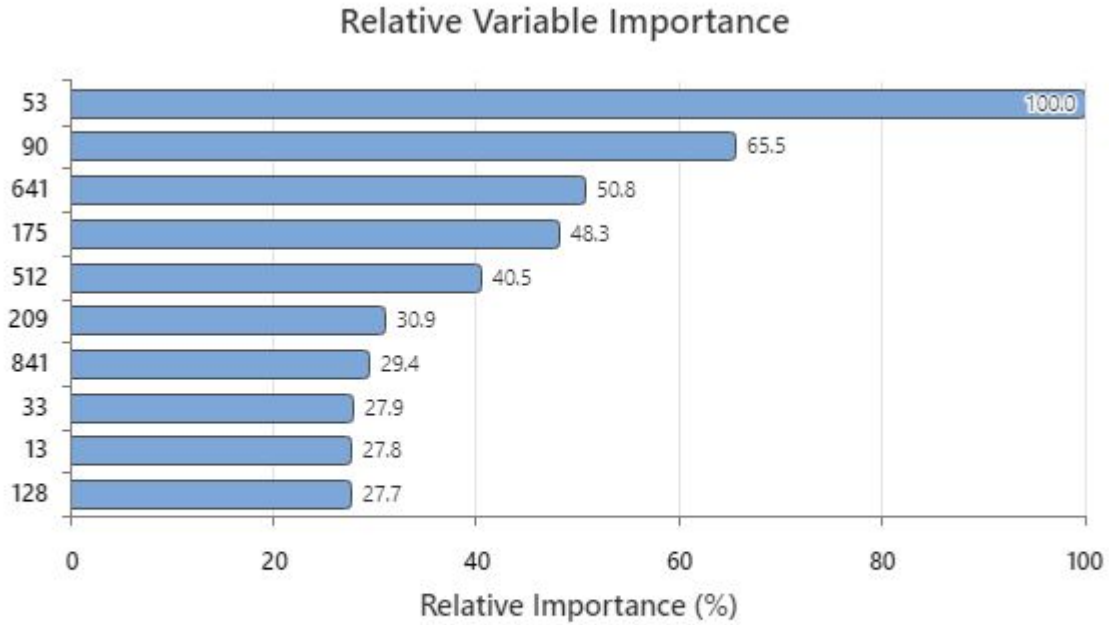
Model	Optimal Number of Trees	Area Under ROC Curve	Number of Predictors	Eliminated Predictors
52	275	0.972072	7	841
53	291	0.972891	6	13
54	299	0.970147	5	209
55	144	0.960278	4	175
56	2	0.853726	3	512
57	1	0.779402	2	90
58	1	0.75561	1	641

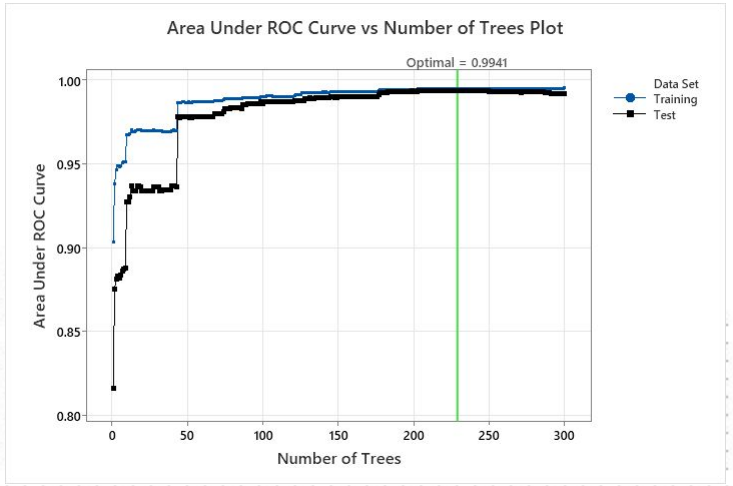
Discovering the 10-Marker Model

Model Summary

Total predictors	10
Important predictors	10
Number of trees grown	300
Optimal number of trees	229

Statistics	Training	Test
Average -loglikelihood	0.0527	0.0628
Area under ROC curve	0.9949	0.9941
95% CI	(0.9913, 0.9985)	(0.9880, 1)
Lift	9.4206	9.6125
Misclassification rate	0.0162	0.0252





- The entire discovery process is finished in minutes!

Case Study 3: Predicting Drug Toxicity

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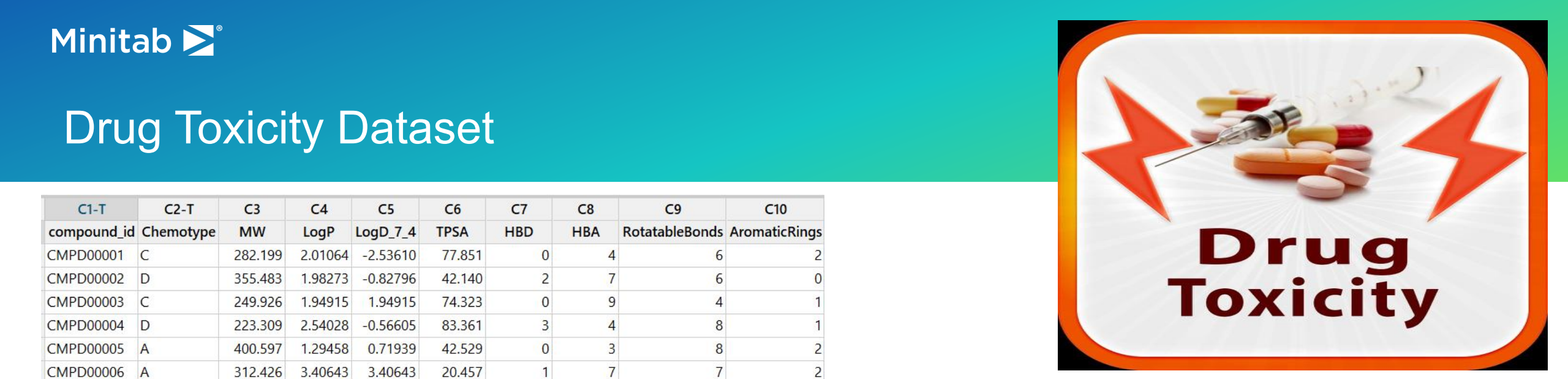
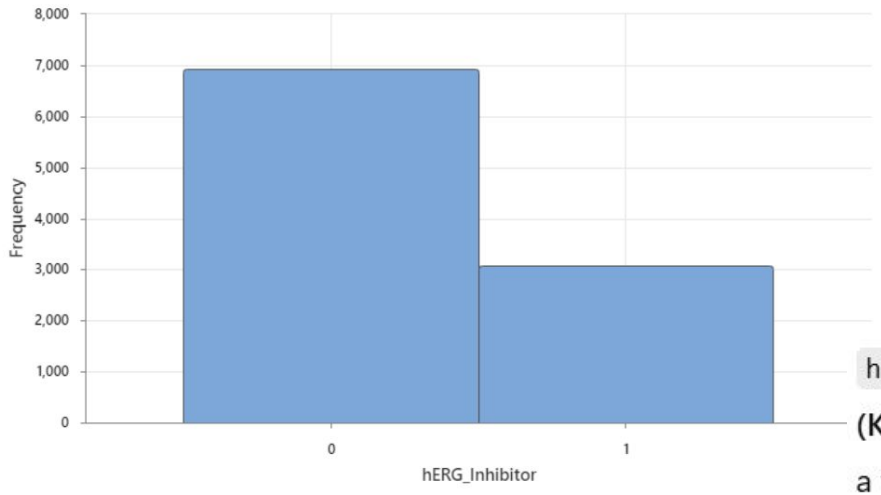
Drug Toxicity Dataset

C1-T	C2-T	C3	C4	C5	C6	C7	C8	C9	C10
compound_id	Chemotype	MW	LogP	LogD_7_4	TPSA	HBD	HBA	RotatableBonds	AromaticRings
CMPD00001	C	282.199	2.01064	-2.53610	77.851	0	4	6	2
CMPD00002	D	355.483	1.98273	-0.82796	42.140	2	7	6	0
CMPD00003	C	249.926	1.94915	1.94915	74.323	0	9	4	1
CMPD00004	D	223.309	2.54028	-0.56605	83.361	3	4	8	1
CMPD00005	A	400.597	1.29458	0.71939	42.529	0	3	8	2
CMPD00006	A	312.426	3.40643	3.40643	20.457	1	7	7	2





- A dataset containing 10000 drug trial compounds
  - 6 binary target responses related to toxicity and efficacy
  - 30 categorical and continuous predictors describing the molecular structure and chemical characteristics of each compound
- Want to understand what factors correlate with different types of toxicity

`hERG_Inhibitor` is a **binary flag** indicating whether a compound is predicted to **inhibit the cardiac hERG (KCNH2) potassium channel**. Inhibition of hERG reduces the I_Kr current, can **prolong the QT interval**, and is a well-known **cardiotoxicity liability** (linked to torsades de pointes).

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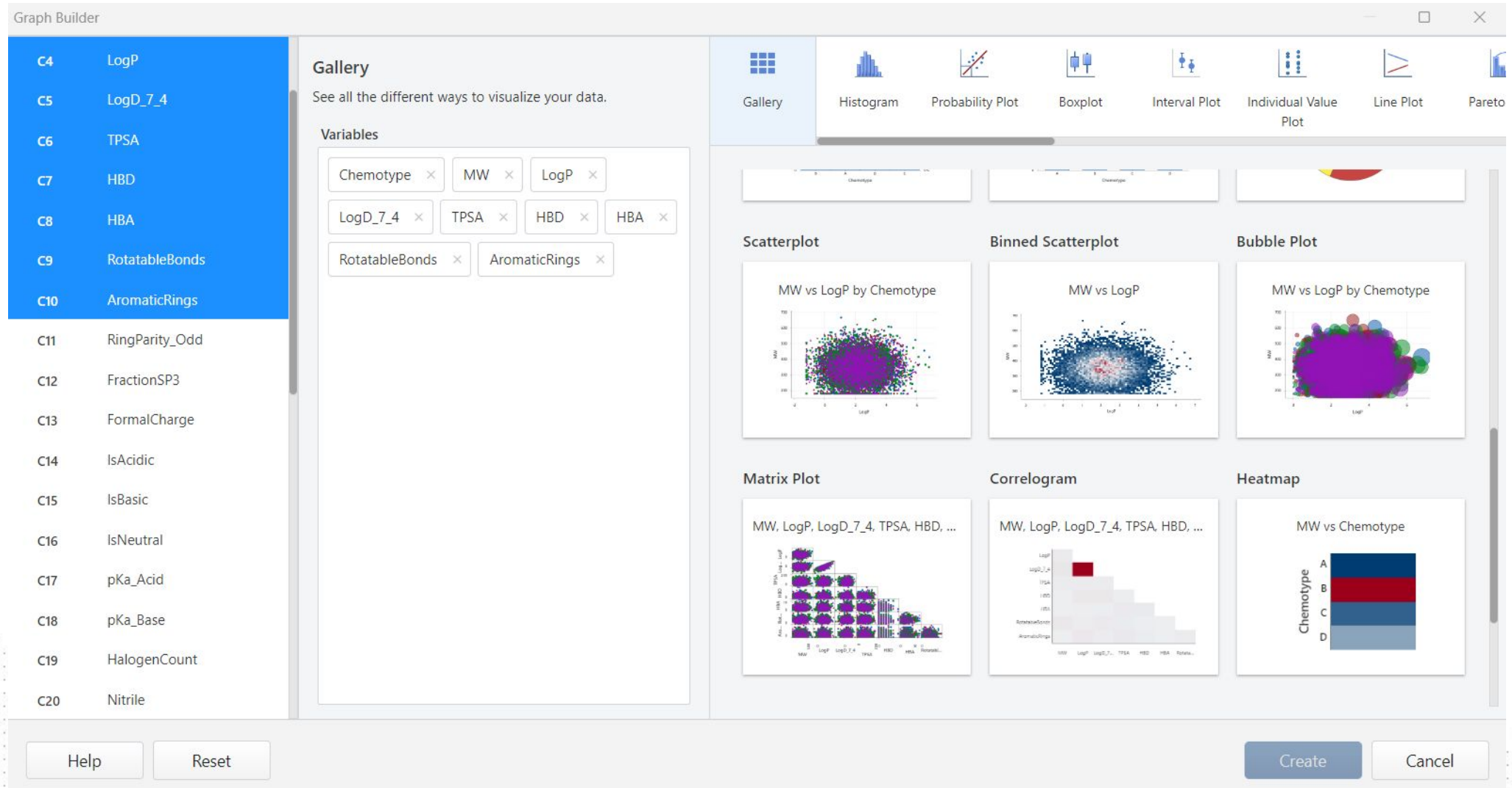
Descriptive AI



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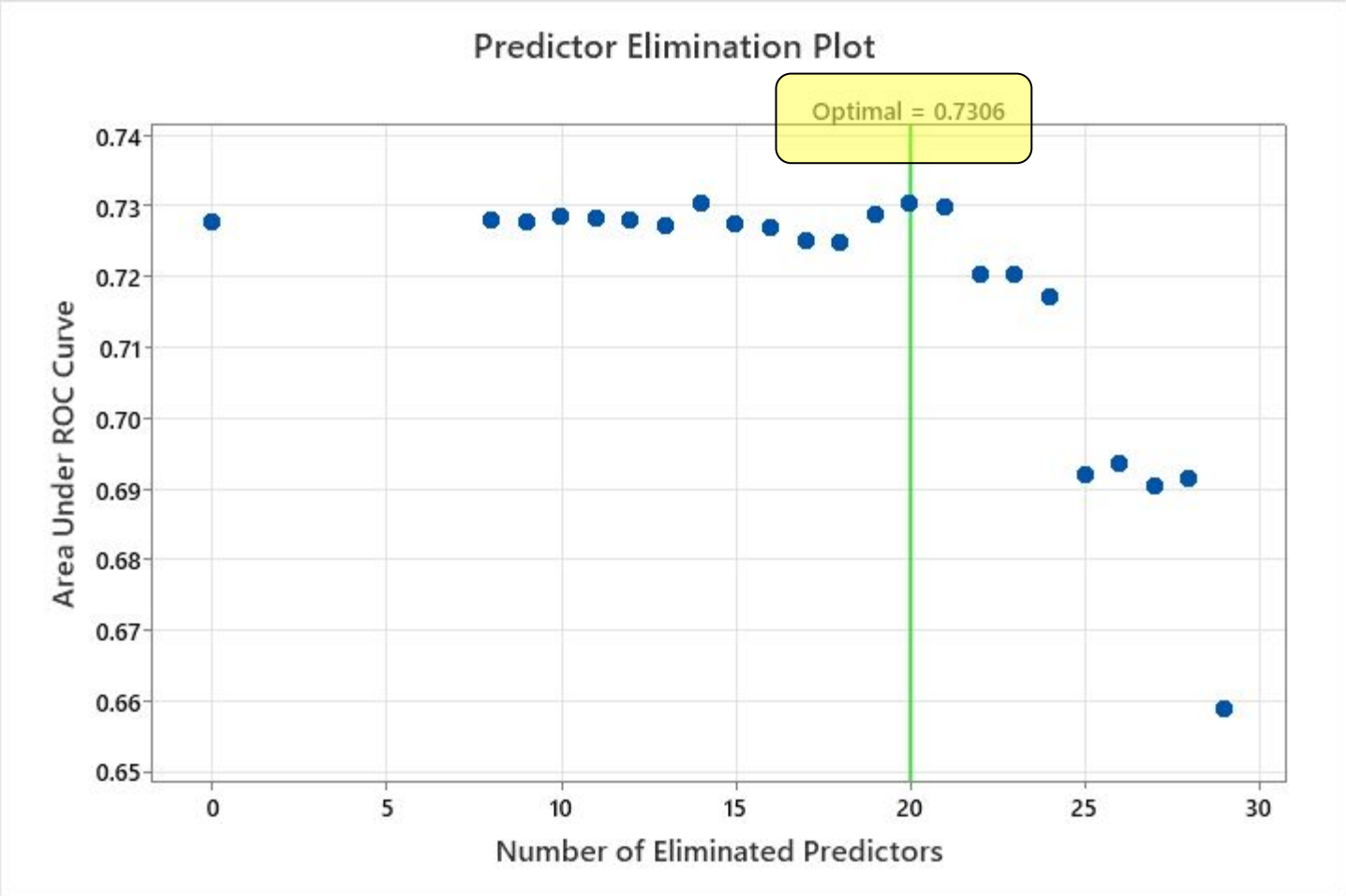
Predictor Discovery AI



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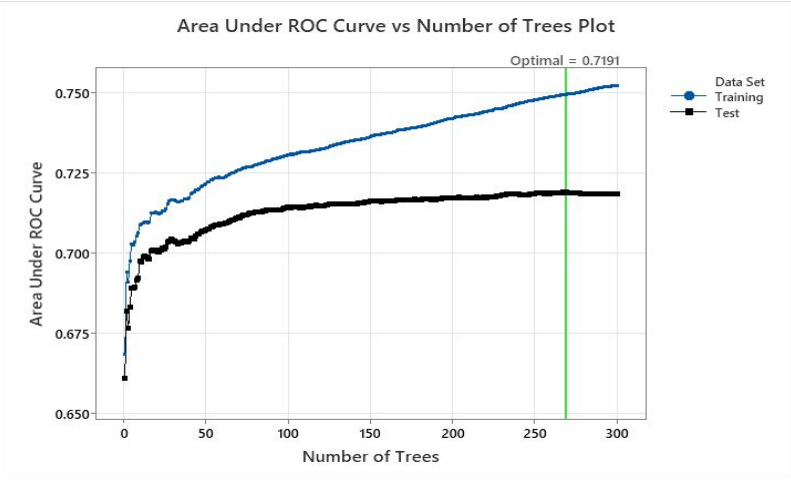
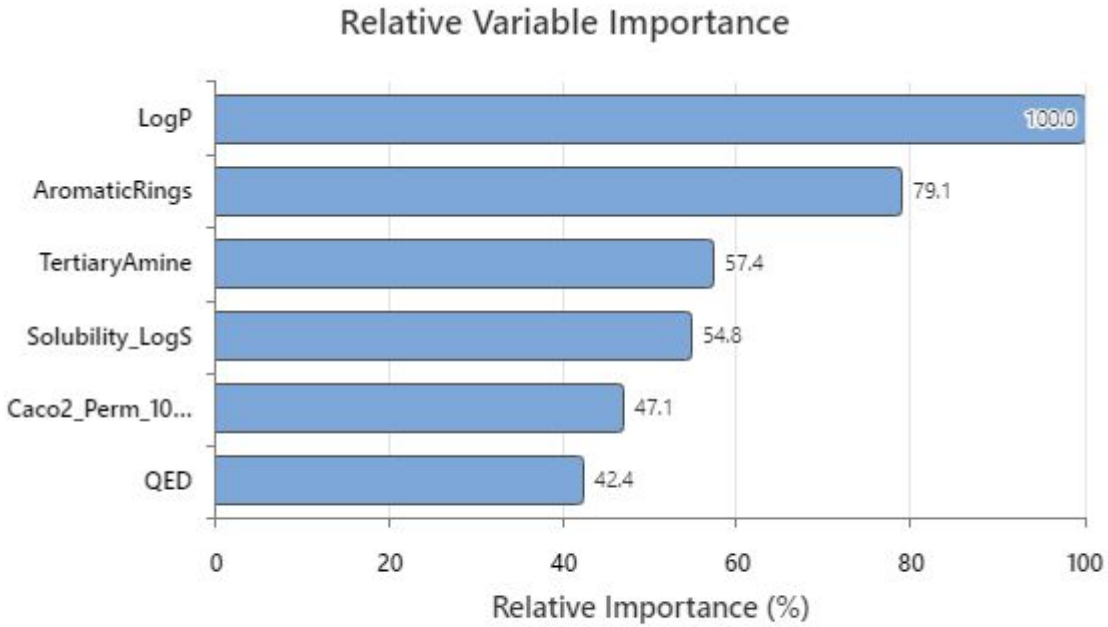
The Final Model Candidate

Model Summary

Total predictors	6
Important predictors	6
Number of trees grown	300
Optimal number of trees	269

Statistics	Training	Test
Average -loglikelihood	0.5324	0.5462
Area under ROC curve	0.7496	0.7191
95% CI	(0.7373, 0.7618)	(0.6993, 0.7388)
Lift	2.3734	2.1359
Misclassification rate	0.2631	0.2712





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Predictors of Interest

- **LogP** is a measure of a molecule's **lipophilicity** (how "fat-loving" or hydrophobic it is).
- **AromaticRings** (in the dataset) is an **integer count** of how many **aromatic rings** a compound has.
- **TertiaryAmine** (in the dataset) is a **binary flag (0/1)** that marks whether the compound contains a **tertiary amine functional group**.
- **Solubility_LogS** is the **base-10 logarithm of aqueous solubility expressed in mol/L** (molar solubility):
- **Caco2_Perm_10e6cms** is the **Caco-2 apparent permeability** (**Papp**) measured across a Caco-2 cell monolayer, reported in **units of 10−610^{-6}10−6 cm/s**.
- **QED** stands for **Quantitative Estimate of Drug-likeness**. It's a single number in **[0, 1]** that summarizes how "drug-like" a **small-molecule** is based on a handful of simple physicochemical properties. Higher is more drug-like *by this heuristic*.

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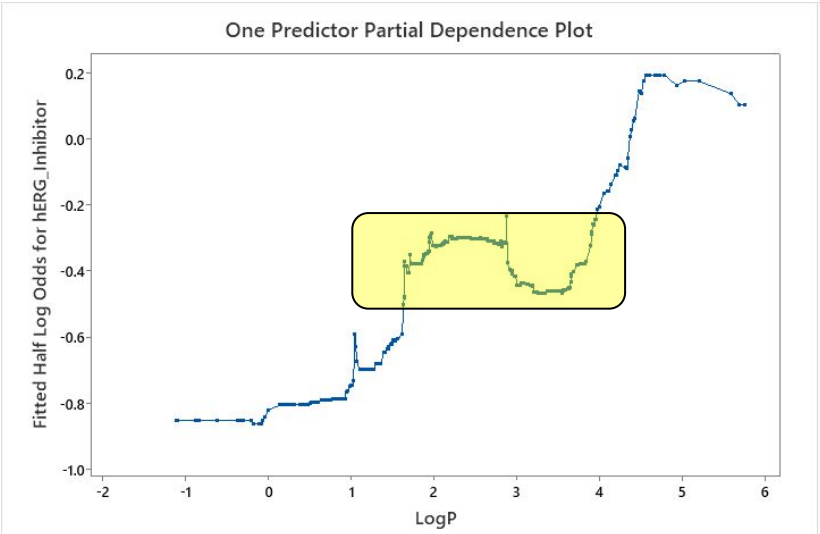
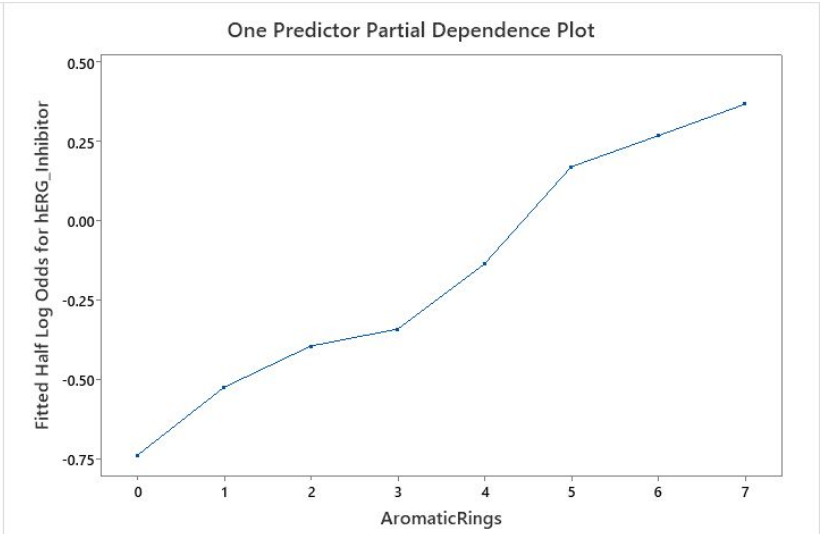
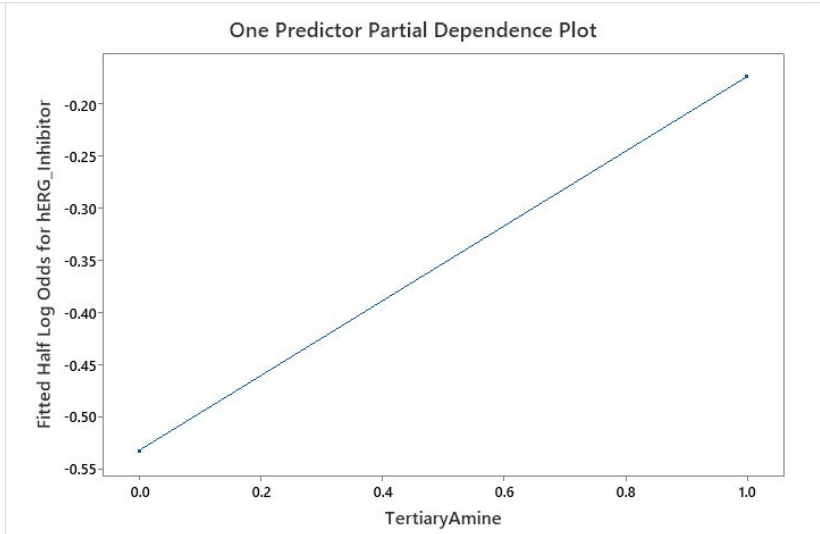
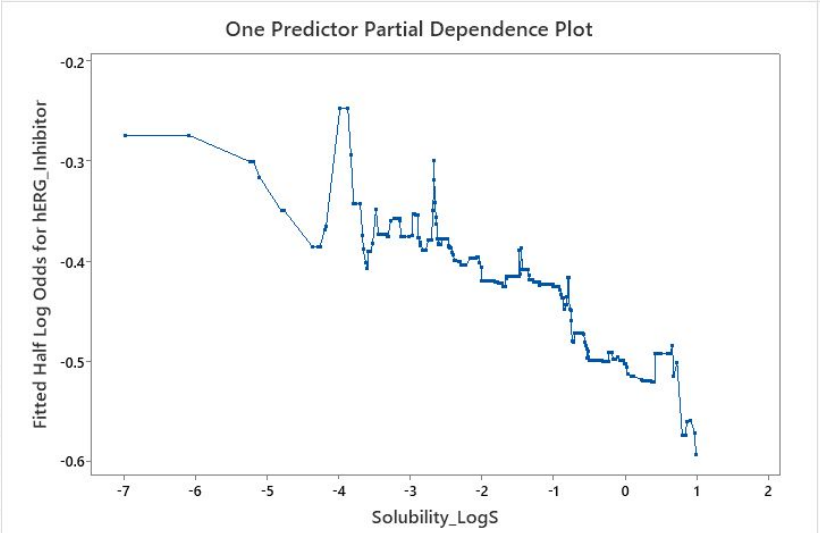
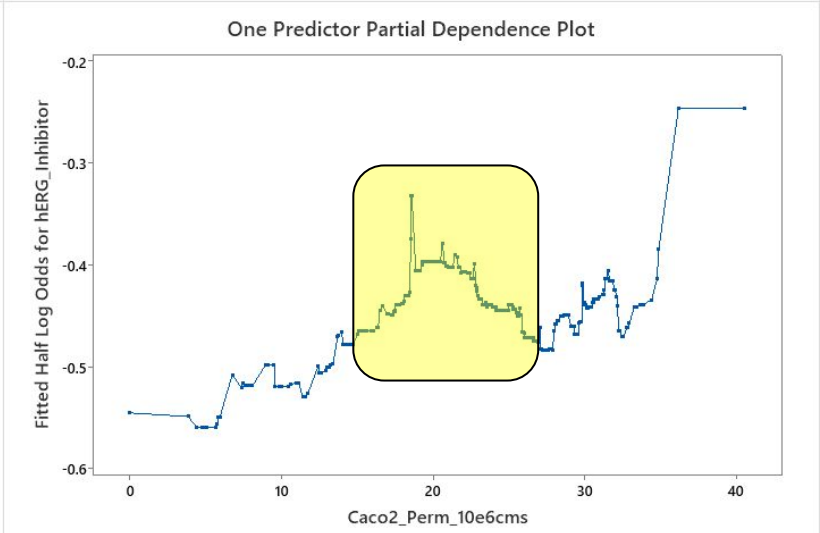
TN Model Interpretation

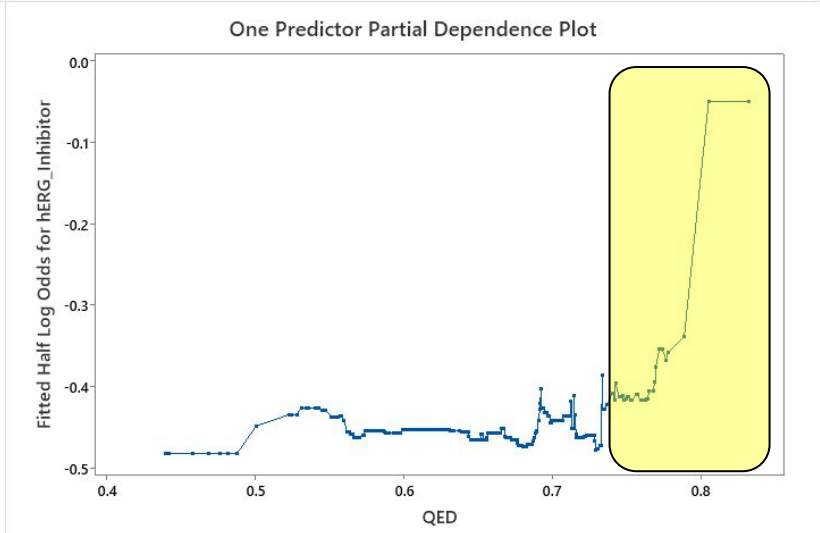












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Logistic Regression Model

Model Summary

Deviance R-Sq	Deviance R-Sq(adj)	AIC	AICc	BIC	Area Under ROC Curve	Test Deviance R-Sq	Test Area Under ROC Curve
9.96%	9.89%	7798.17	7798.19	7846.15	0.7070	8.58%	0.6935

Coefficients

Term	Coef	SE Coef	Z-Value	P-Value	VIF
Constant	-4.372	0.344	-12.70	0.000	
LogP	0.3451	0.0599	5.76	0.000	5.95
AromaticRings	0.3506	0.0214	16.37	0.000	1.05
TertiaryAmine	0.8924	0.0622	14.35	0.000	1.01
QED	2.414	0.495	4.88	0.000	1.05
Solubility_LogS	-0.0578	0.0553	-1.04	0.296	7.00
Caco2_Perm_10e6cms	0.00947	0.00463	2.04	0.041	1.47

Regression Equation

$$P(1) = \exp(Y')/(1 + \exp(Y'))$$

$$Y' = -4.372 + 0.3451\ \text{LogP} + 0.3506\ \text{AromaticRings} + 0.8924\ \text{TertiaryAmine} + 2.414\ \text{QED} - 0.0578\ \text{Solubility\_LogS} + 0.00947\ \text{Caco2\_Perm\_10e6cms}$$

- Comments:
  - Reduced model performance (0.69 vs 0.72)
  - Global monotone structure
  - AI already did all the predictor discovery heavy lifting

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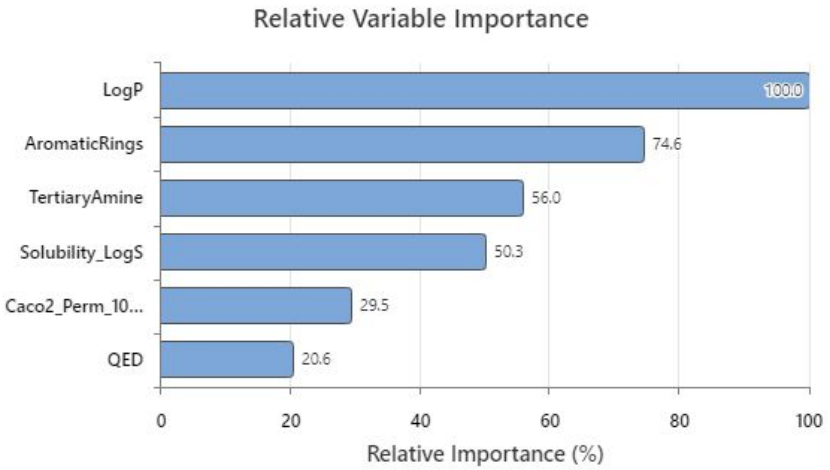
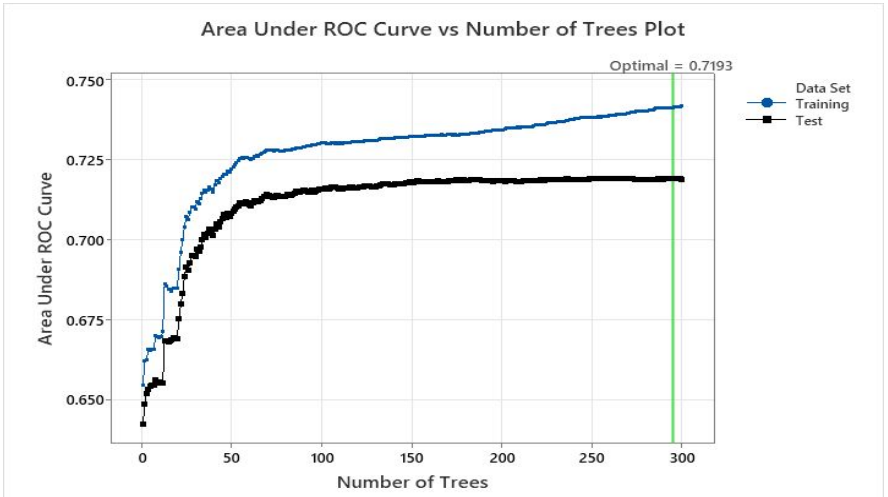
Assessing the Impact of Interactions

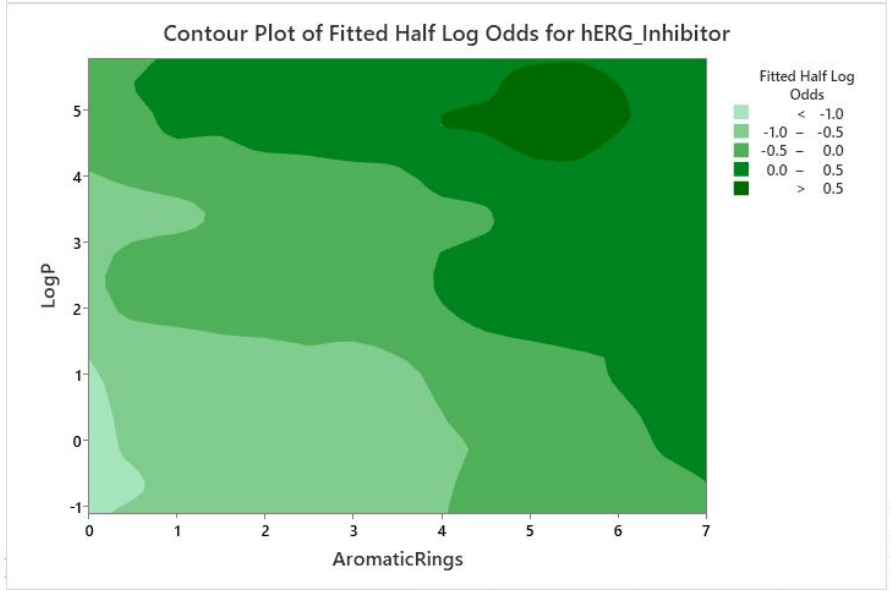
Model Summary

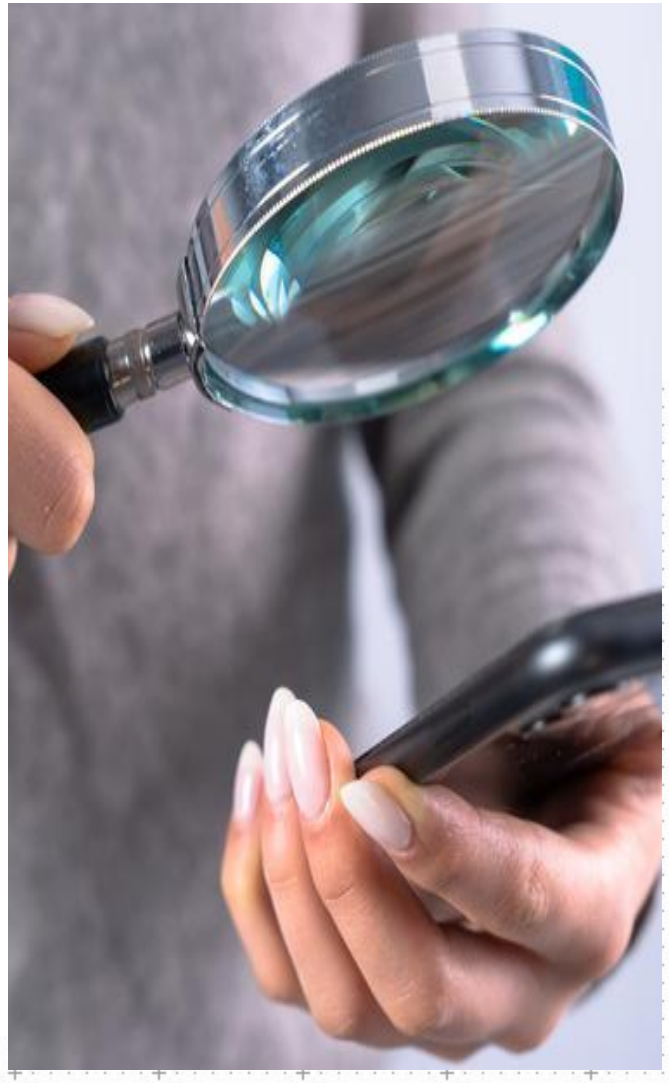
Total predictors	6
Important predictors	6
Number of trees grown	300
Optimal number of trees	295

Statistics	Training	Test
Average -loglikelihood	0.5399	0.5463
Area under ROC curve	0.7413	0.7193
95% CI	(0.7289, 0.7537)	(0.6996, 0.7390)
Lift	2.3243	2.1105
Misclassification rate	0.2668	0.2735









Generative AI

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What About Generative AI?

- **Reactive Machines:**
  - These are basic rule-based systems that operate based on predefined rules.
- **Expert Systems:**
  - These are computer systems that mimic the decision-making ability of a human expert in a specific domain.
- **Machine Learning (ML) Systems:**
  - ML is a subset of AI that focuses on developing algorithms and models that enable computers to learn from data.
  - Types of ML systems include **supervised learning (PA)**, unsupervised learning, and reinforcement learning.
- **Neural Networks:**
  - Inspired by the human brain, neural networks are a key component of many AI systems.
- **Narrow/Generative AI (Weak AI):**
  - These AI systems are designed and trained for a specific task or a narrow set of tasks.
  - Examples include virtual personal assistants, image recognition software, and language translation services.

Text In
Text Out

- **Limited Memory:**
  - These AI systems can learn from historical data to make better decisions.
  - Self-driving cars often use limited memory AI to navigate based on past experiences.
  - Can be integrated into robots to enable them to learn and interact with the environment.
- **Self-aware AI:**
  - This refers to hypothetical AI systems with self-awareness and consciousness.
- **Theory of Mind:**
  - This is a more advanced form of AI that can understand human emotions, beliefs, intentions, and thoughts.
- **General AI (Strong AI):**
  - General AI systems can understand, learn, and apply knowledge across diverse domains.
  - They can perform any intellectual task that a human being can do.
- **Superintelligent AI:**
  - This is a theoretical AI that surpasses human intelligence in every aspect.

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A More General Case of PA

Text In
Text Out

- To engage in **Generative AI**, you **must have**:
- **Clear Problem Definition** – **predict** Output Text **based on** Input Text
- **Historical Dataset** – a fixed corpus of documents
- Due to the special nature of the historical dataset (unstructured text), the target predictors requirements have been generalized:
  - **Response/Target variable** – Output Text
  - **Predictor variables** – Input Text

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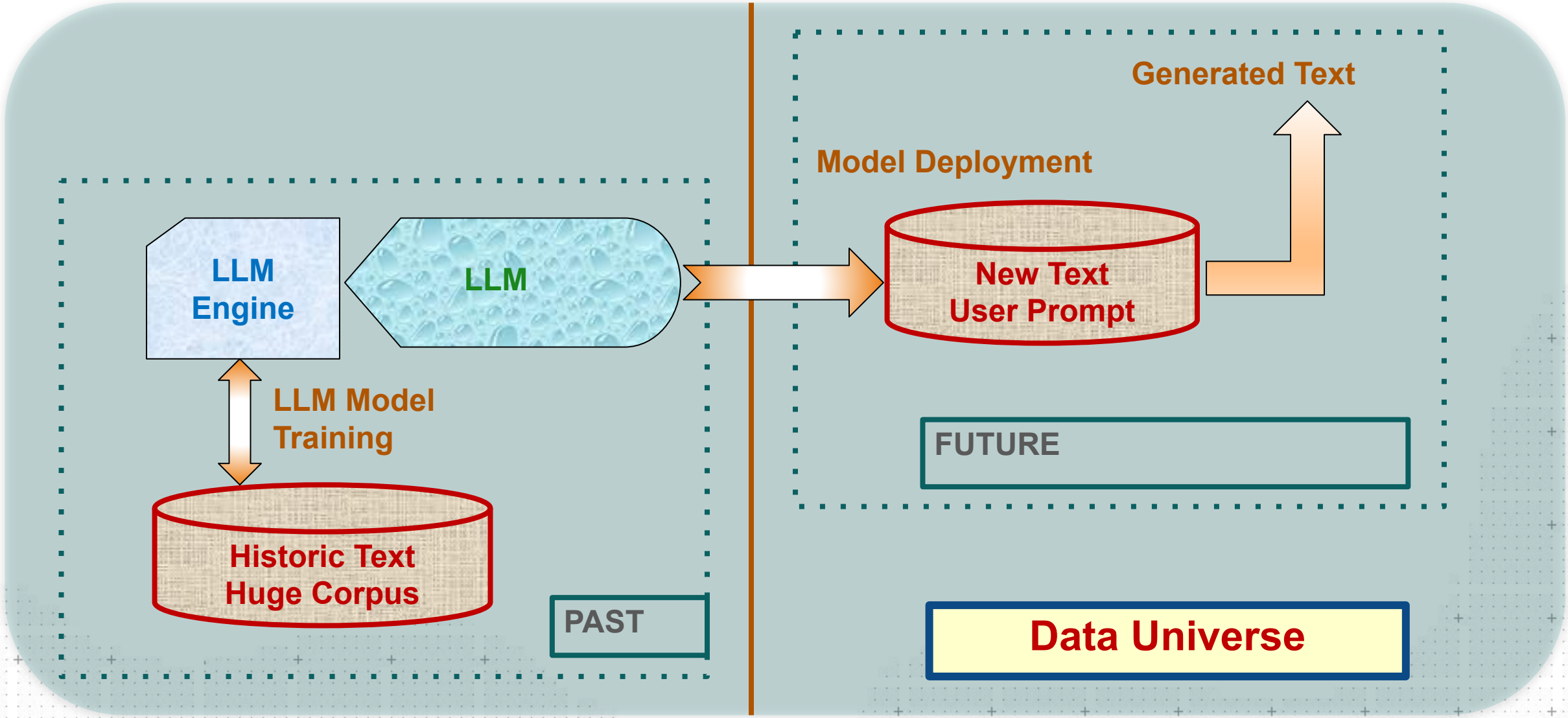
Large Language Model Process (Gen AI)



Generations of Information Retrieval (IR)

- Libraries
  - As old as ancient Greece and Egypt
  - Culminated in the Library of Congress Classification
- Pre-digital Mechanization (19th-20th centuries: index cards, punch cards, etc.)
- Early Computerized IR (1940s-1960s: Boolean searches, etc.)
- Search Databases (1970s-1980s: electronic abstracts, indices, etc.)
- Web-search era (1990s-2000s: Web Crawler, Alta Vista, Yahoo, Google, etc.)
- Big Data and ML (2010s: collaborative filtering, recommender systems, personal assistants, etc.)
- Generative AI and Conversational Retrieval (2020s: ChatGPT and its likes)

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How Should We Handle Generative AI?

Divination

Interrogation

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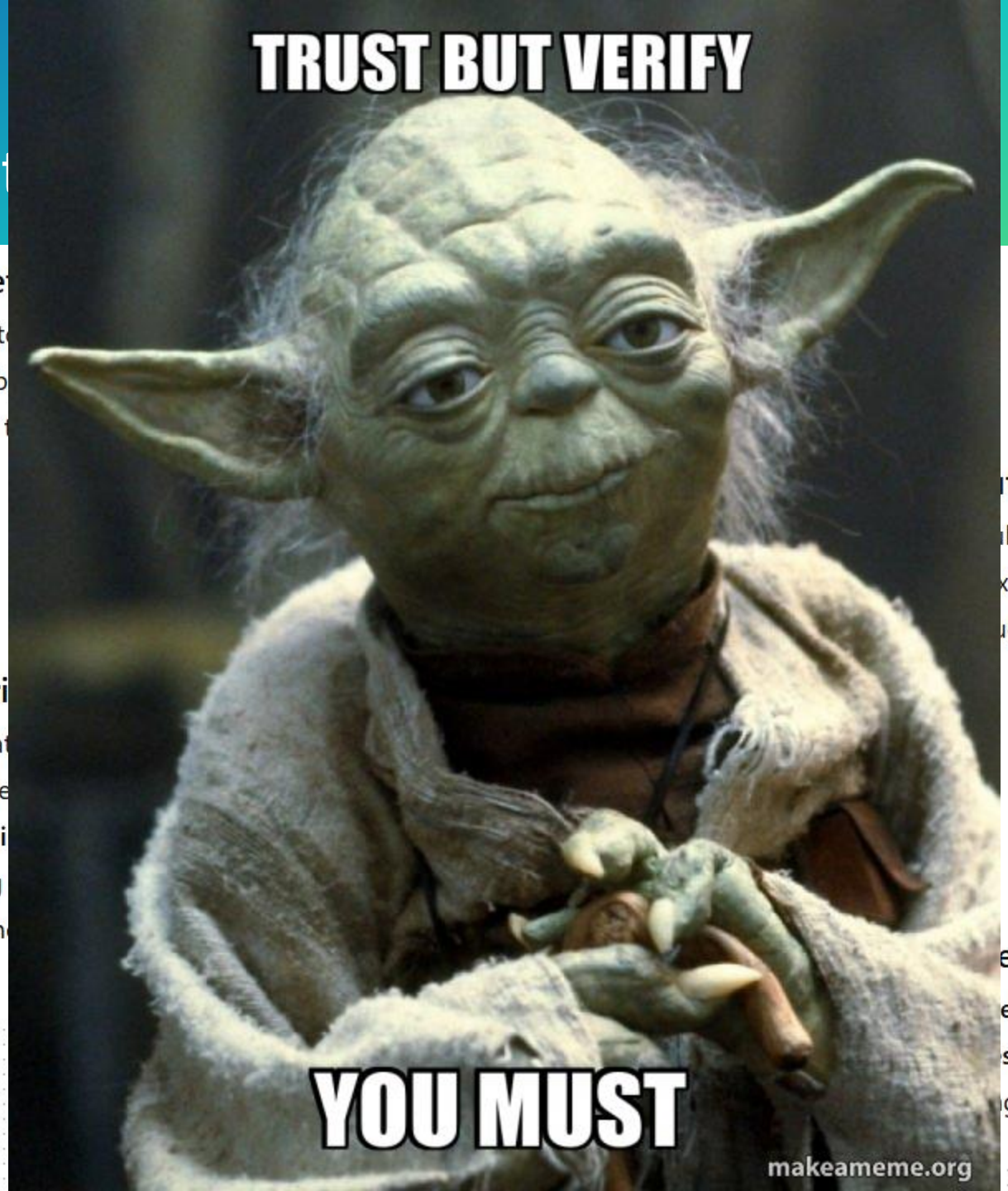
Examples of Chat

1. Fabricated Legal Precedents & Def

- In **May 2023**, a lawyer submitted a brief t
  precedents that were entirely generated b
  conduct, noting the fraudulent nature of t

3. Fabricated Biographical, Histori

- ChatGPT has produced wildly inaccurat
  - Claiming Leonardo da Vinci painte
  - Stating that **George Washington i**
  - Creating fake academic-sounding
    which even fooled experts until th



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xicity. The AI gave this advice
ugh to be reported in a medical

e Summaries

er found that AI tools—including ChatGPT—
s, and produce misleading summaries. One
g users to reliable sources, making fact-

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GenAI Fundamental Flaws

- The end of scalability with the release of GPT 5.0 (Moore's law yielding to the 90/10 rule)
- Creation vs Regurgitation
- Unacceptable Liability (Code Generation vs Medical Advice)
- Hacking and code/prompt injection attacks
- Emotional attachments
- Mega Hitler phenomenon and other ethical issues
  - Ghosting
  - Red-lining
- "Don't Hallucinate" oxymoron
- Flooding the Data Universe with the superfluous (garbage) content
  - Junk books on Amazon (book mills)
  - Junk science papers (paper mills)
  - Junk reviews and bots (content mills)

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Data Driven Problem Solving

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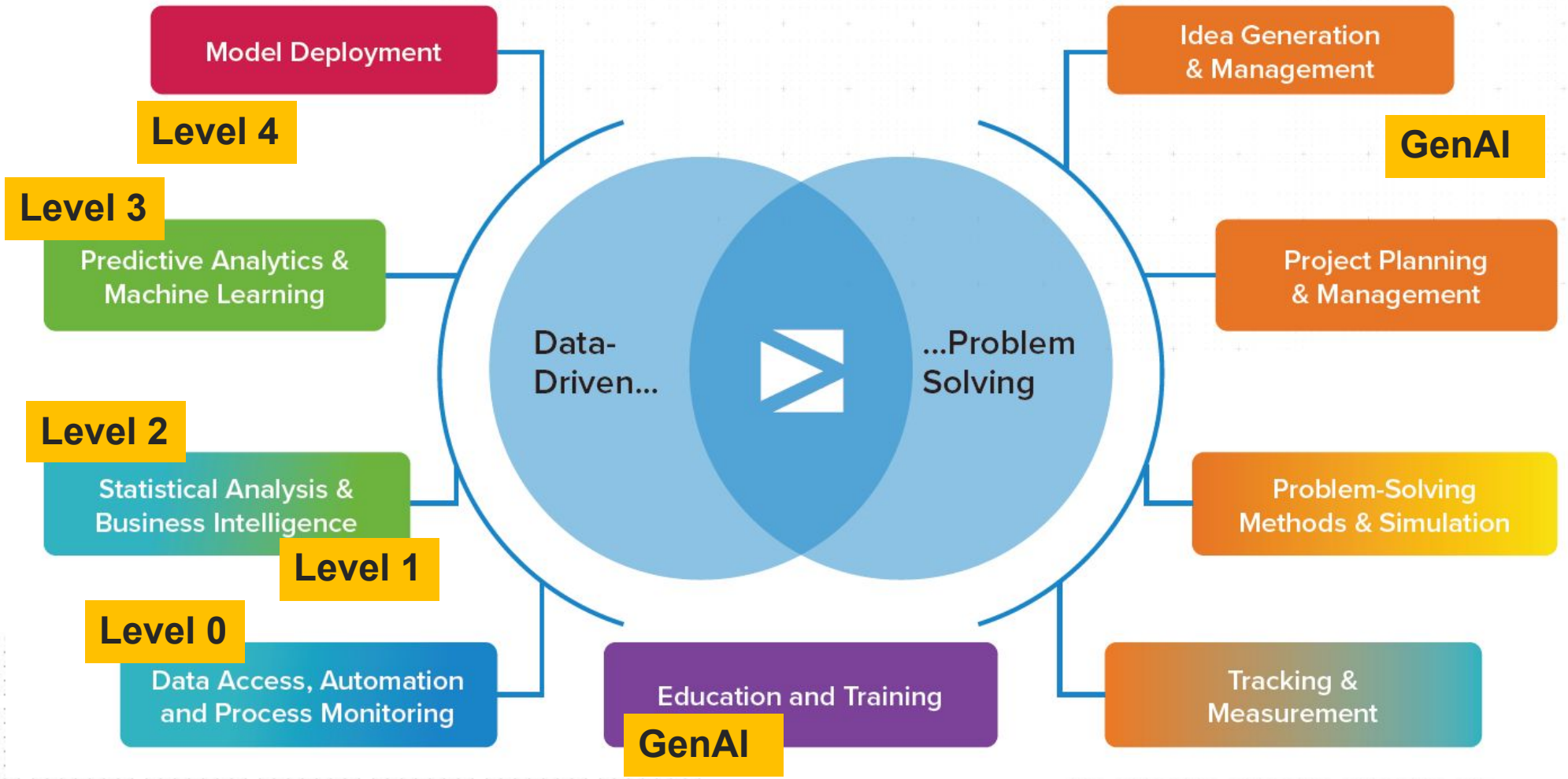
A Suite of Solutions



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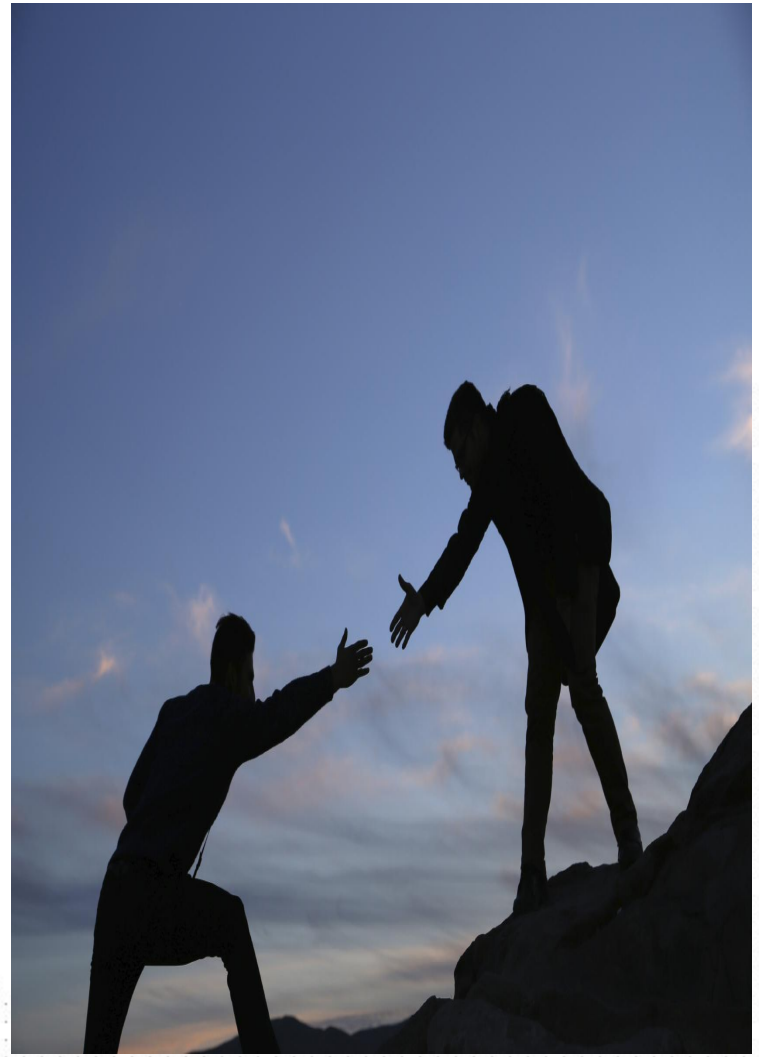
Why Minitab?

- Trusted “down to Earth” digital transformation tools and techniques
- Realistic innovation in data science and machine learning
- Focus on understanding your business needs and offering practical data-driven solutions
- Versatile project-management tools, both individual and corporate
- Variety of data access, data gathering, and data storage tools
- Real-time sensor-based process monitoring
- Intuitive descriptive statistics, graphs, control charts, and dashboards
- State of the art powerful machine learning algorithms
- Scalable model deployment and model monitoring facilities
- Discrete event simulation tools
- Python, R, and ChatGPT connectors
- Information and education aids to bring you up to speed



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- In this presentation, Mikhail will break down the complexities of modern AI into digestible concepts, making the subject accessible to all. He will then illustrate the key points with an insightful case study from medical research. The following topics will be discussed:
  - The fundamental principles of AI and machine learning.
  - Analyst-driven vs data-driven paradigms in machine learning.
  - A case study to highlight the usefulness of predictive AI in medical research.

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You have data.

[analytics]
[dashboards]
[machine learning]
We have **Solutions Analytics™.**
[training]
[visualizations]
[innovation]

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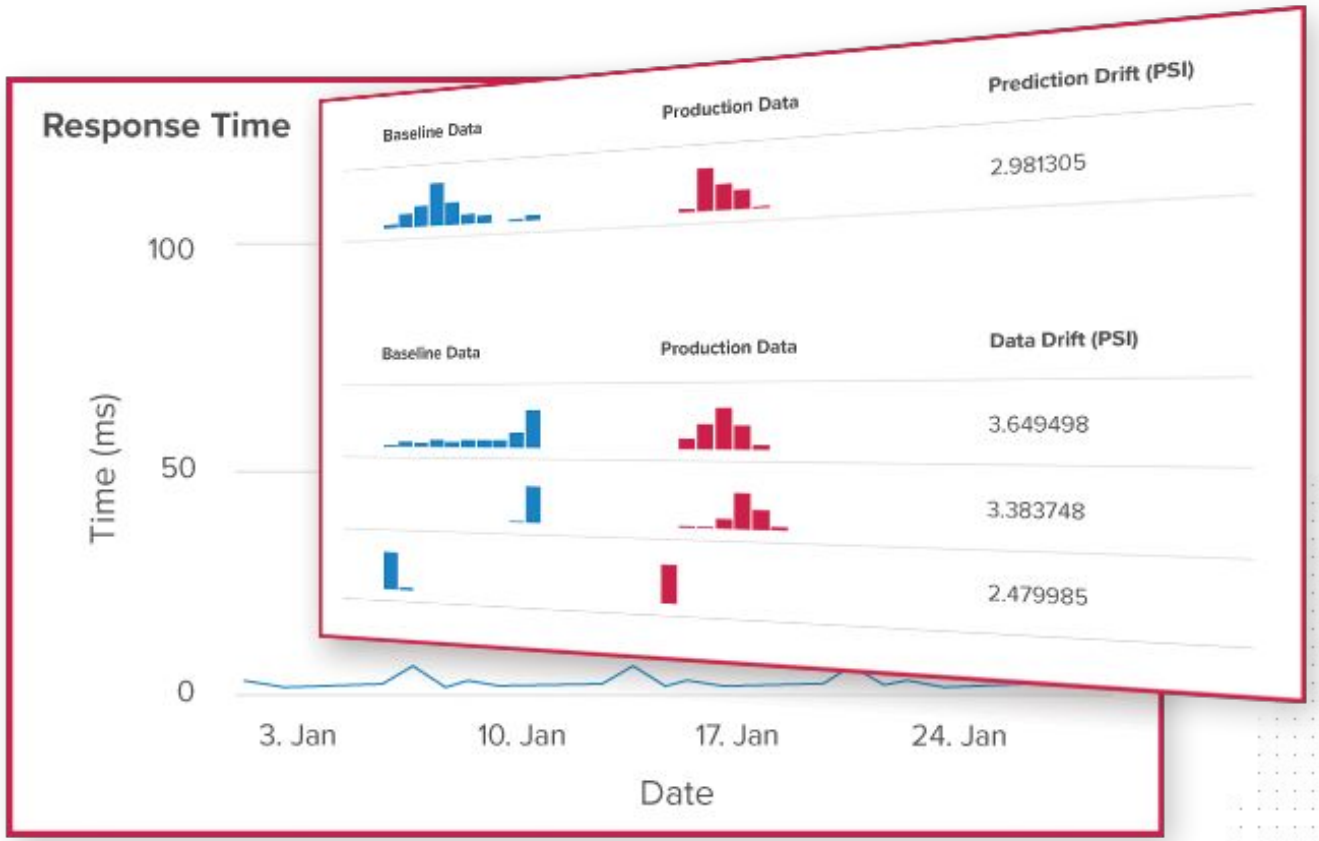

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thank you

Gracias	ευχαριστώ	Danke	Grazie	благодаря
Hvala	Obrigado	Kiitos	شكراً	Tak
Ahsante	Teşekkürler	متشكرم	Salamat Po	감사합니다
Cám ơn	شكريه	Terima Kasih	Dank u Wel	Děkuji
நன்றி	Köszönöm	ありがとうございます	ขอบคุณครับ	Dziękuję
谢谢	Tack	Mulţumesc	спасибо	Merci
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