

# MACHINE LEARNING DESIGN, DEMYSTIFIED

SATURN 2018 Tutorial | May 8 | Plano

**Carnegie Mellon University**  
Software Engineering Institute

**softserve**

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DM18-0886

# INTRODUCTIONS



**Rick Kazman**

Professor, University of Hawaii  
Research Scientist, SEI



**Serge Hazihev**

Head of Intelligent  
Enterprise, SoftServe



**Iurii Milovanov**

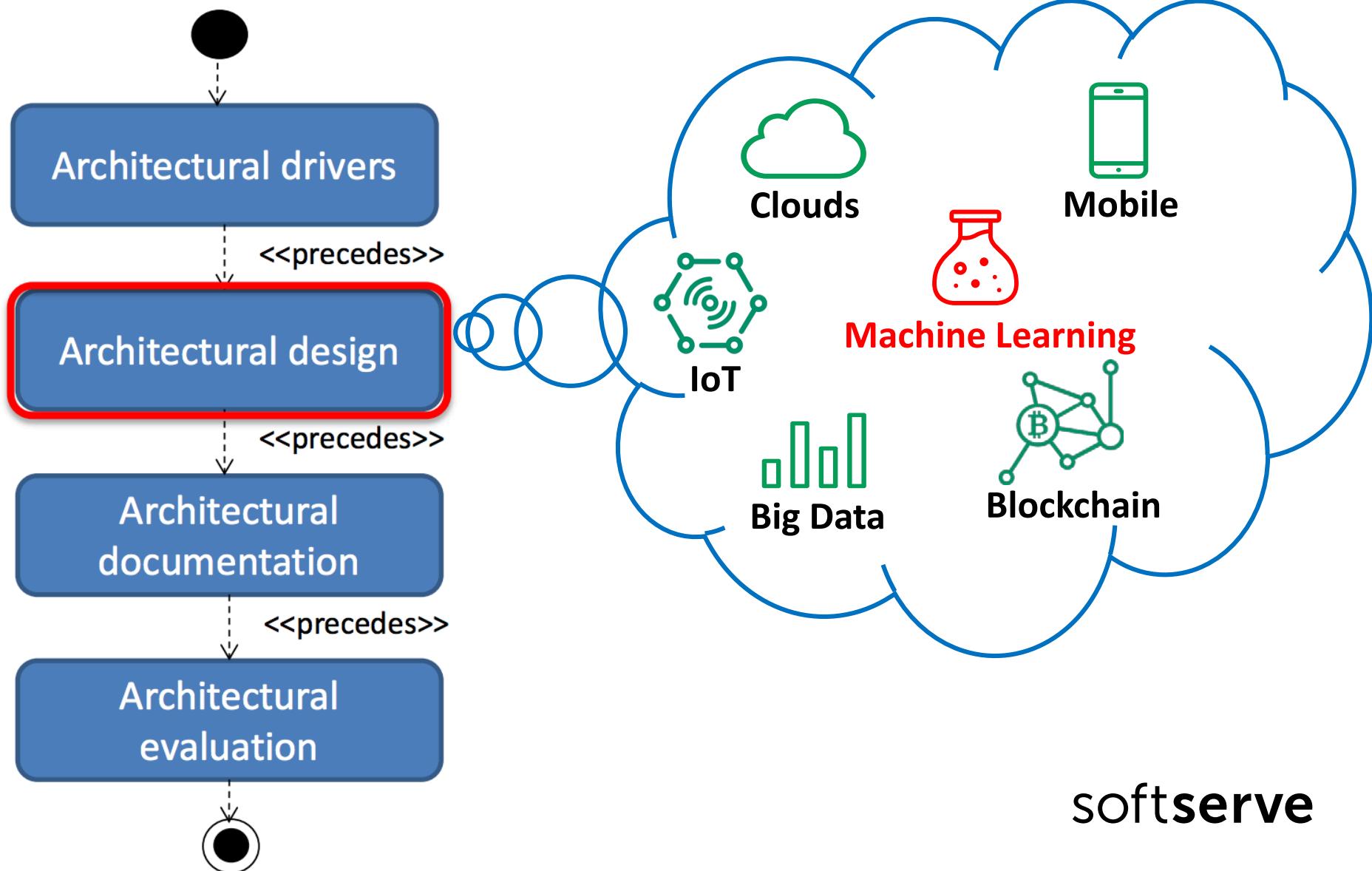
Data Science Practice Leader,  
SoftServe

# AGENDA

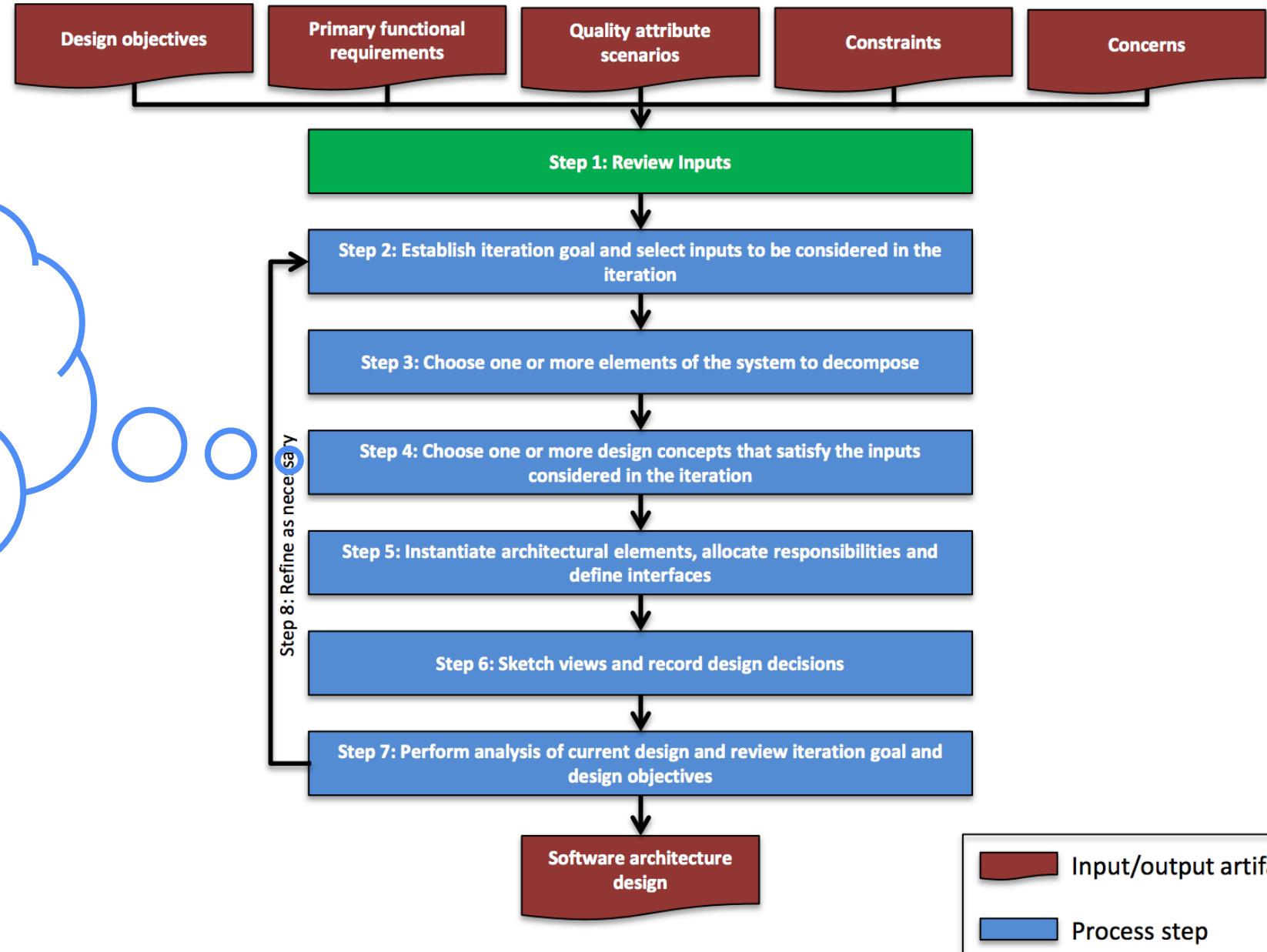
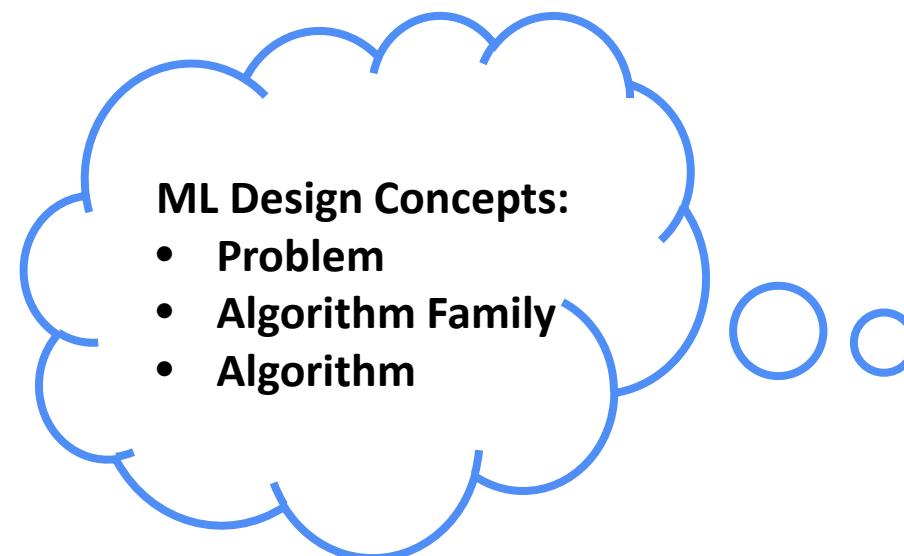
- A Bit of Background
- Game 😊
- Prototyping
- Summary & QA



# MOTIVATION



# ADD 3.0



# SMART DECISIONS GAME

First presented at SATURN 2015

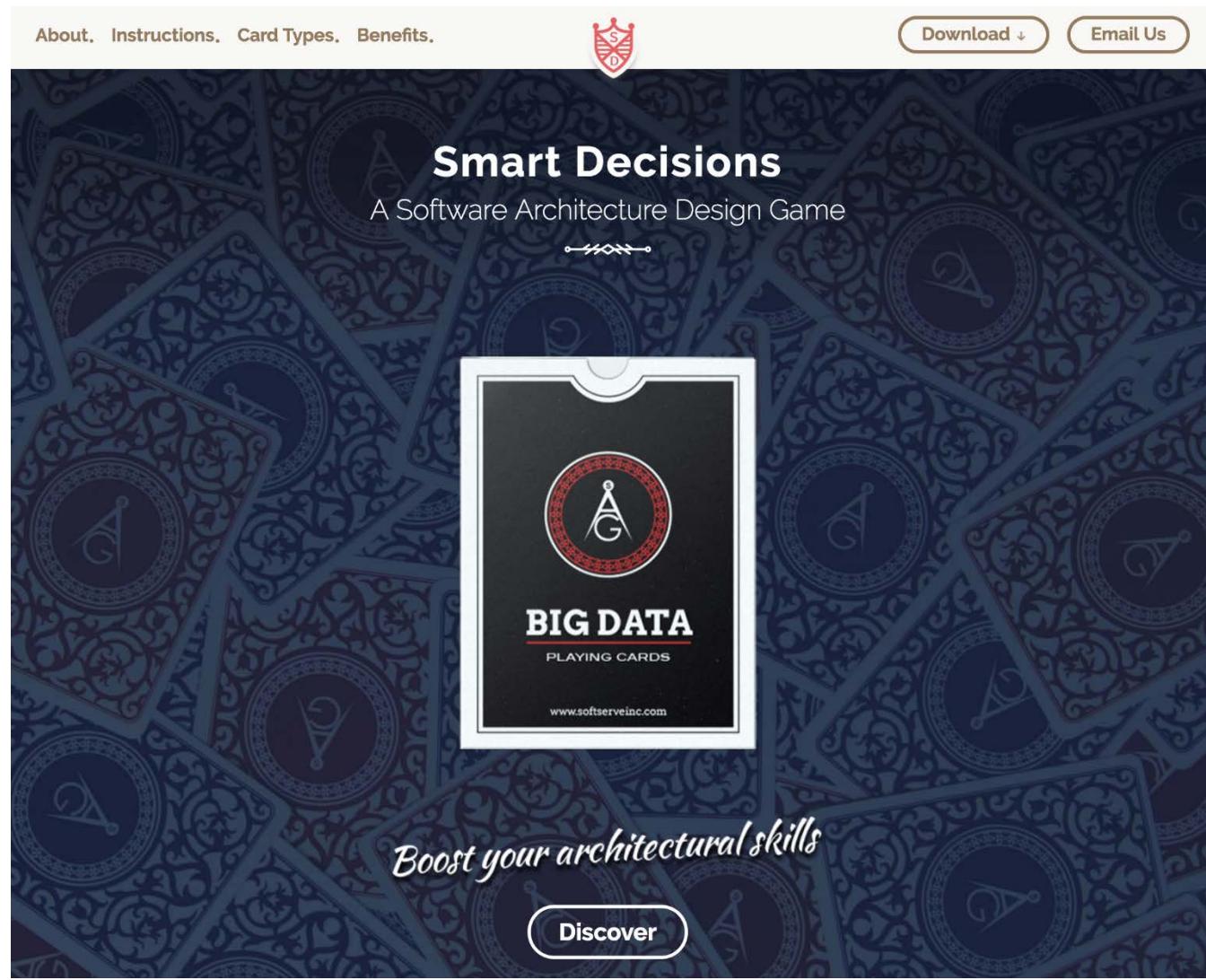
A fun, lightweight way to introduce architectural design and ADD

Available at:

<http://smartdecisionsgame.com/>

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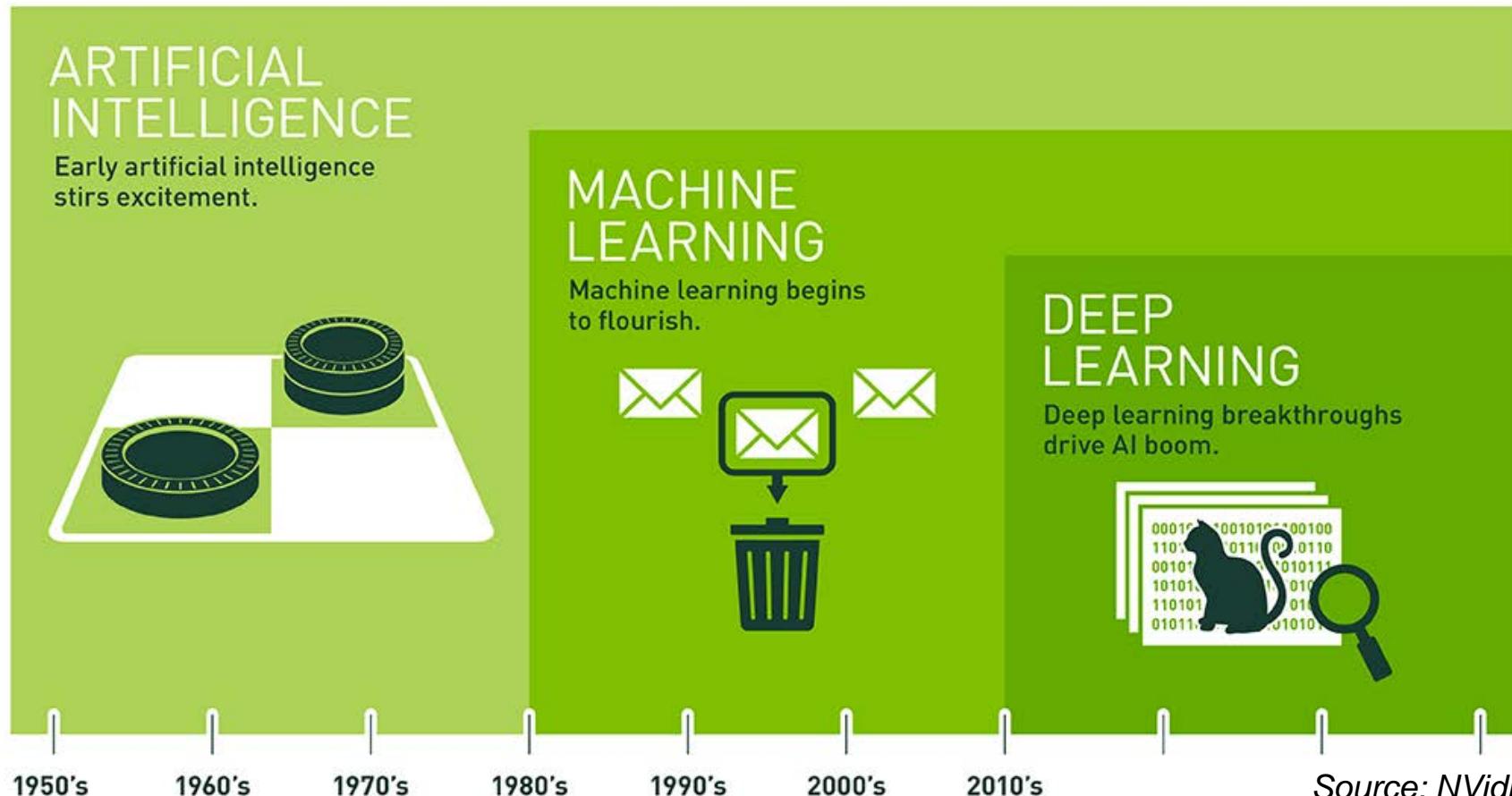
# SHORT QUIZ ☺

What's the name of this company in AI field?

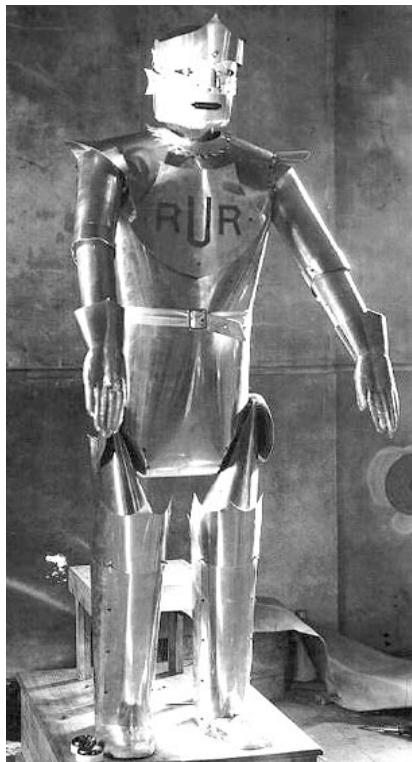
10x increase over the past 2 years!



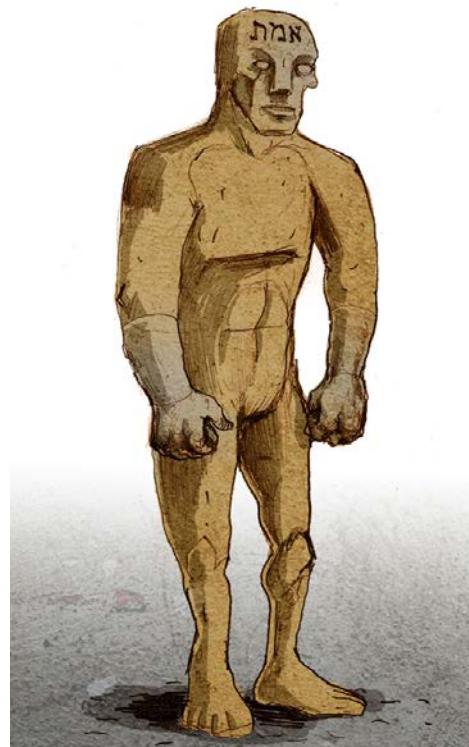
# AI PROGRESS SINCE 1950s



# MYTHS AND FICTION ABOUT ARTIFICIAL BEINGS



R.U.R. (Karel Čapek)  
1921

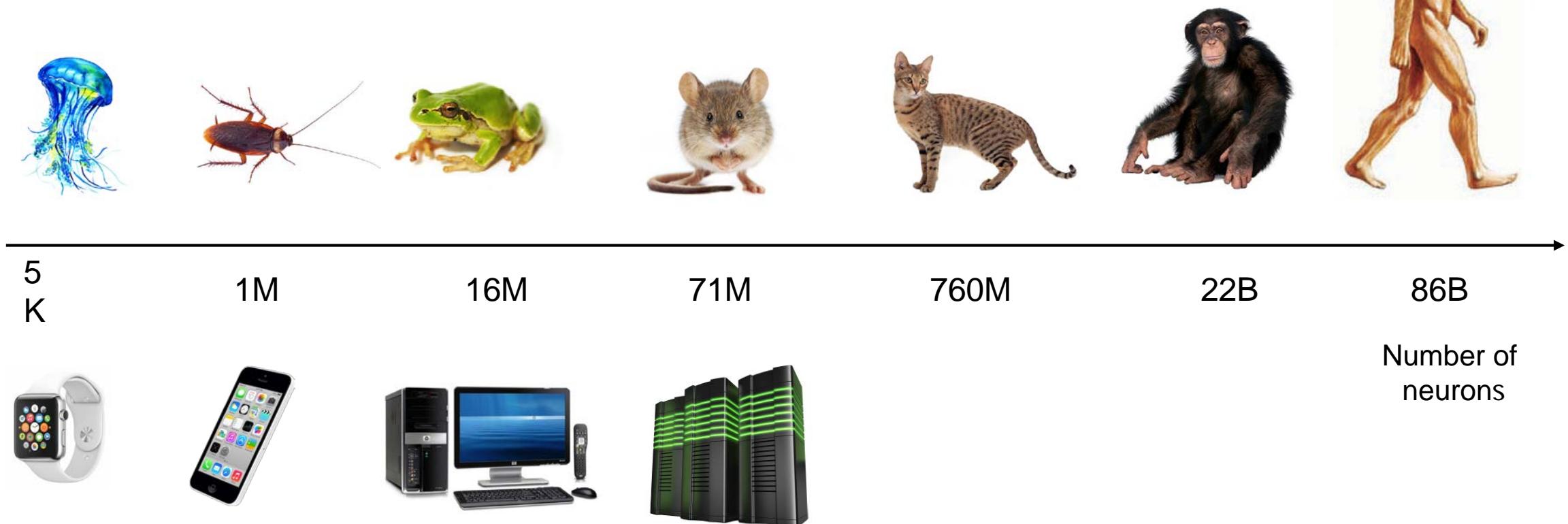


Golem (Bible)  
~1000 BC



Sumerian Anunnaki creating the first man  
~2300 BC

# THE CURRENT STATE OF AI



# GAME CHALLENGE OVERVIEW

## Business Use Case



Banner A



Banner B

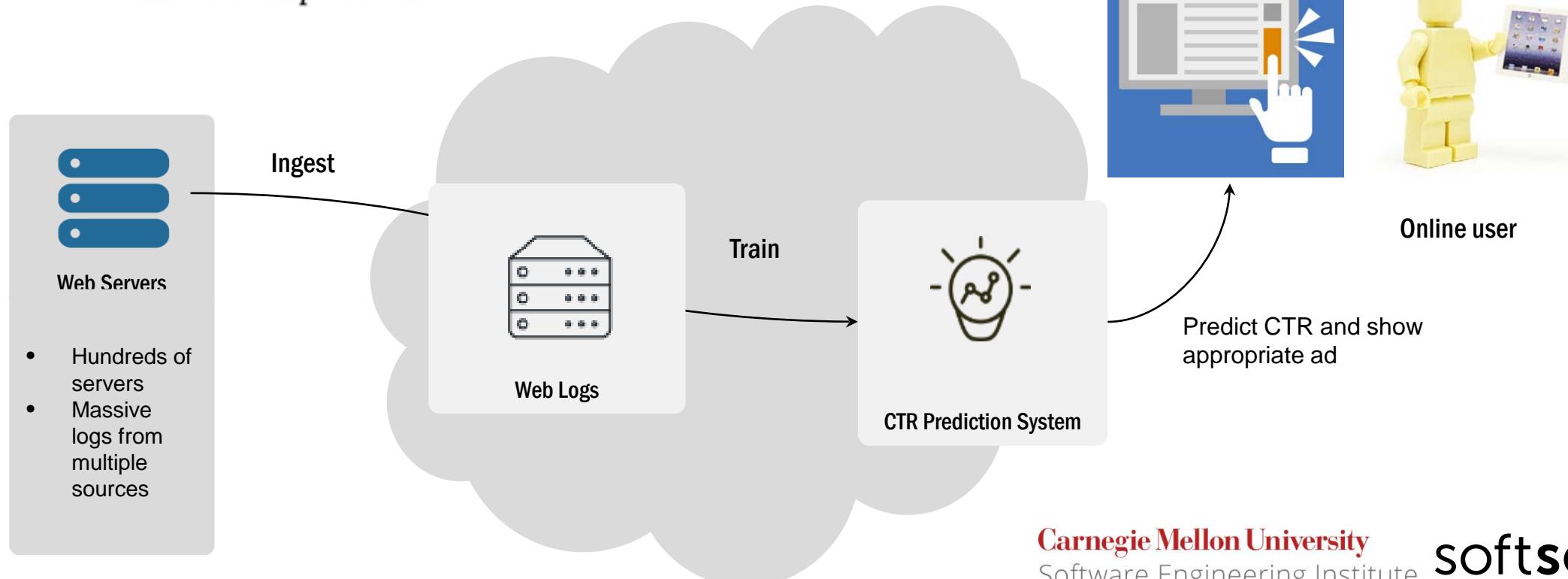
**Which ad will  
the user  
choose?**



# GAME CHALLENGE OVERVIEW

## Marketecture Diagram

$$CTR = \frac{\text{Number of click-throughs}}{\text{Number of impressions}} \times 100(%)$$



# WHY DO WE NEED MACHINE LEARNING?



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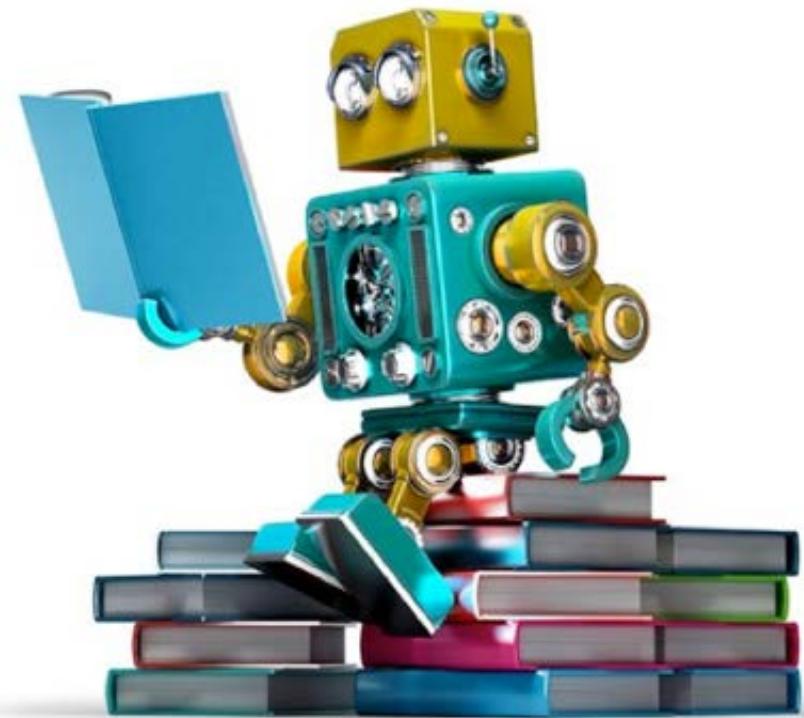
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# WHY NOT JUST CODING?!

**Most of the today's AI problems:**

- Deal with an infinite problem space – think about how many words are there in the English language
- Poorly defined – we still do not know how our brain solves problems

**Therefore, traditional rule-based hand-coding for such problems suffers a 'complexity collapse' and is not feasible**



# MACHINE LEARNING APPROACH

Instead of writing a program by hand, we use a set of examples to train the algorithm

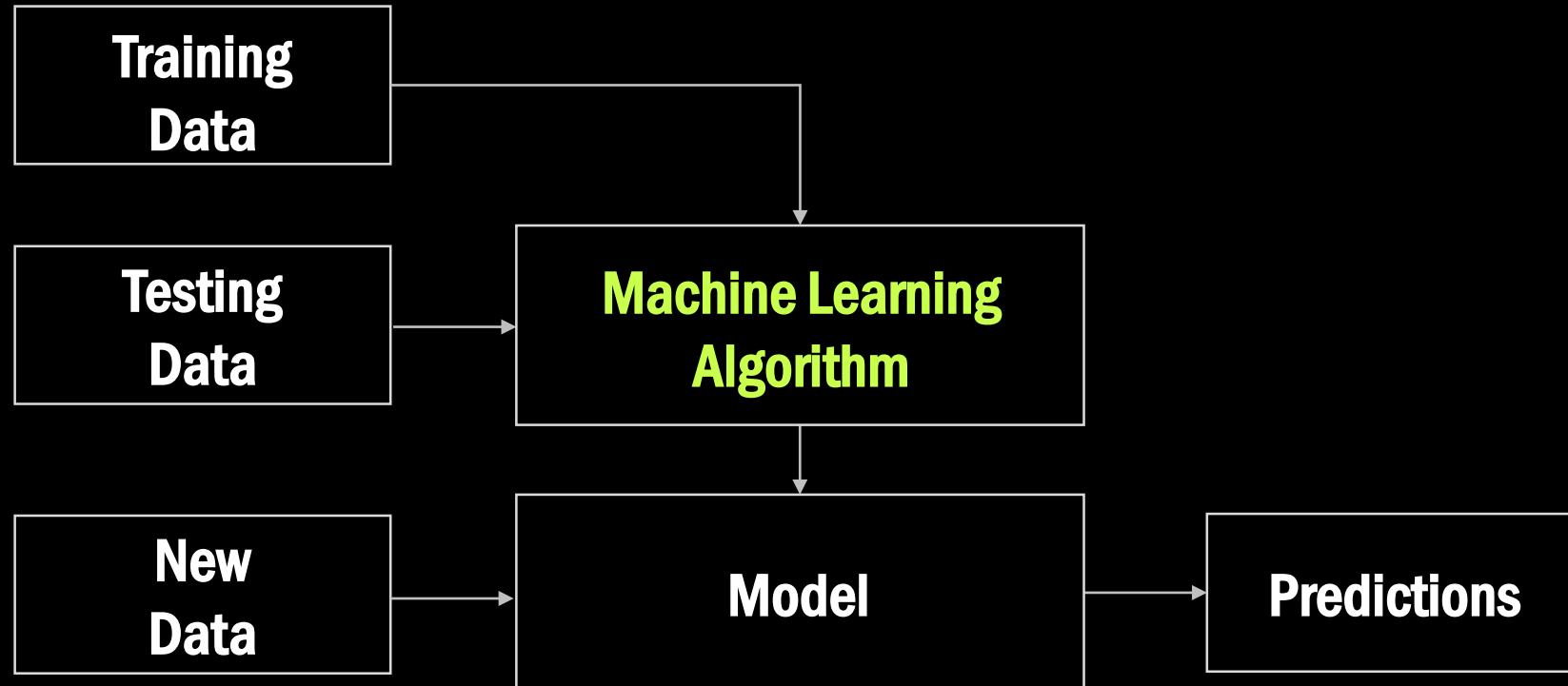


**Developer** writes code



**Algorithm** “writes code”

# ML BUILDING BLOCKS



# TYPES OF LEARNING



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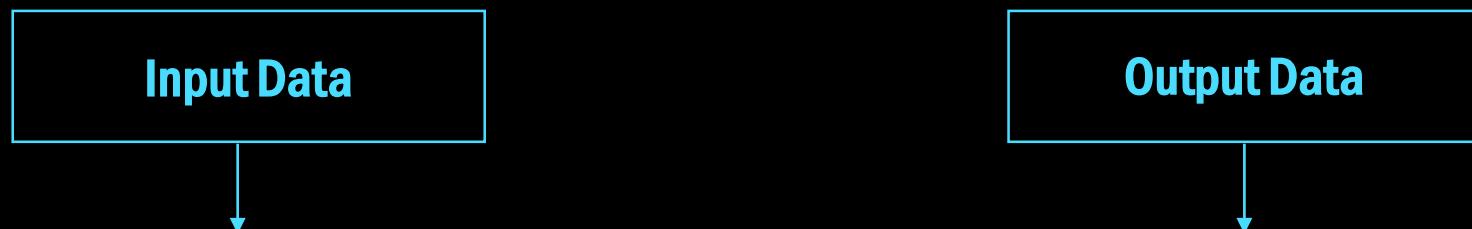
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# SUPERVISED LEARNING

- **Input examples** and corresponding **ground truth outputs** are provided
- The goal is to learn general rules that map a new example to the predicted output



# SUPERVISED LEARNING



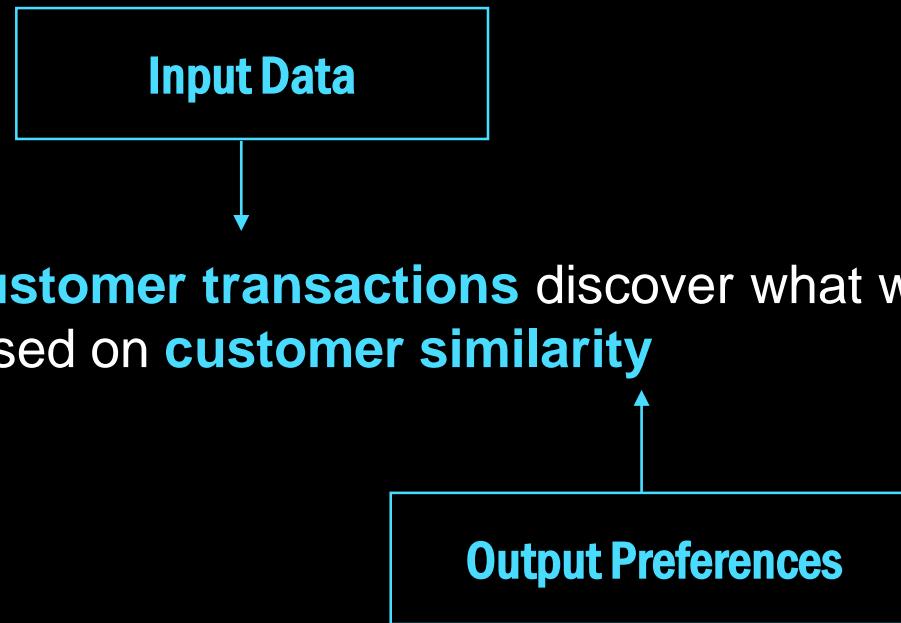
**Example:** Given a set of **house features** along with corresponding **house prices**, predict a price for a new house based on its features (e.g. size, location, etc.)

# UNSUPERVISED LEARNING

- Only **input examples** are provided
- No explicit information about ground truth
- The algorithm tries to discover the internal structure of the data based on some prior knowledge about desired outcome

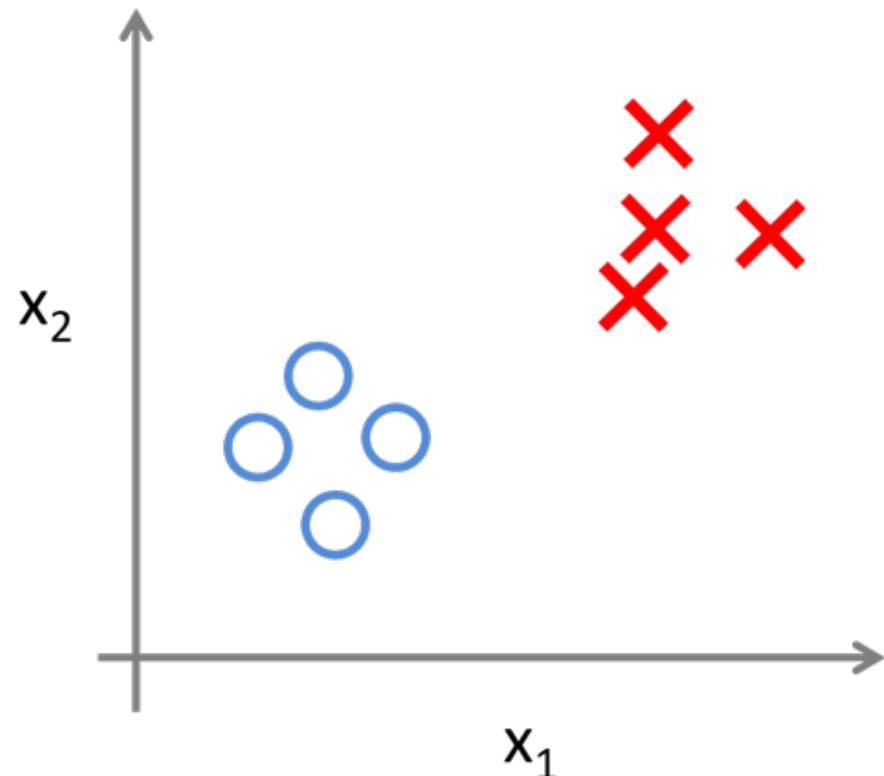


# UNSUPERVISED LEARNING

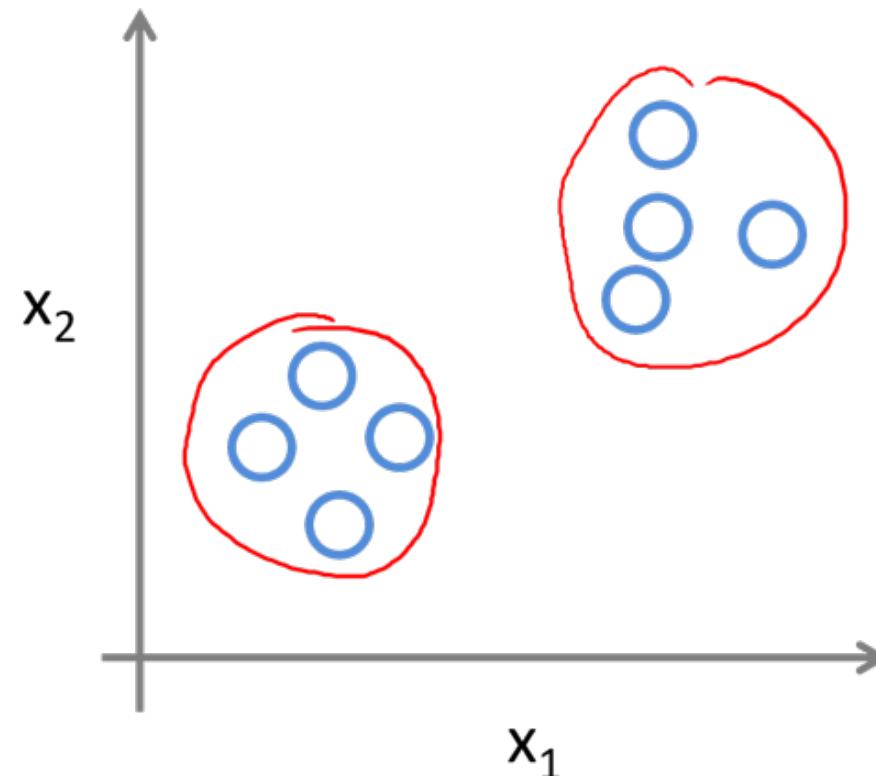


**Example:** Given a set of **customer transactions** discover what would be the best way to group them into clusters based on **customer similarity**

# SUPERVISED LEARNING



# UNSUPERVISED LEARNING

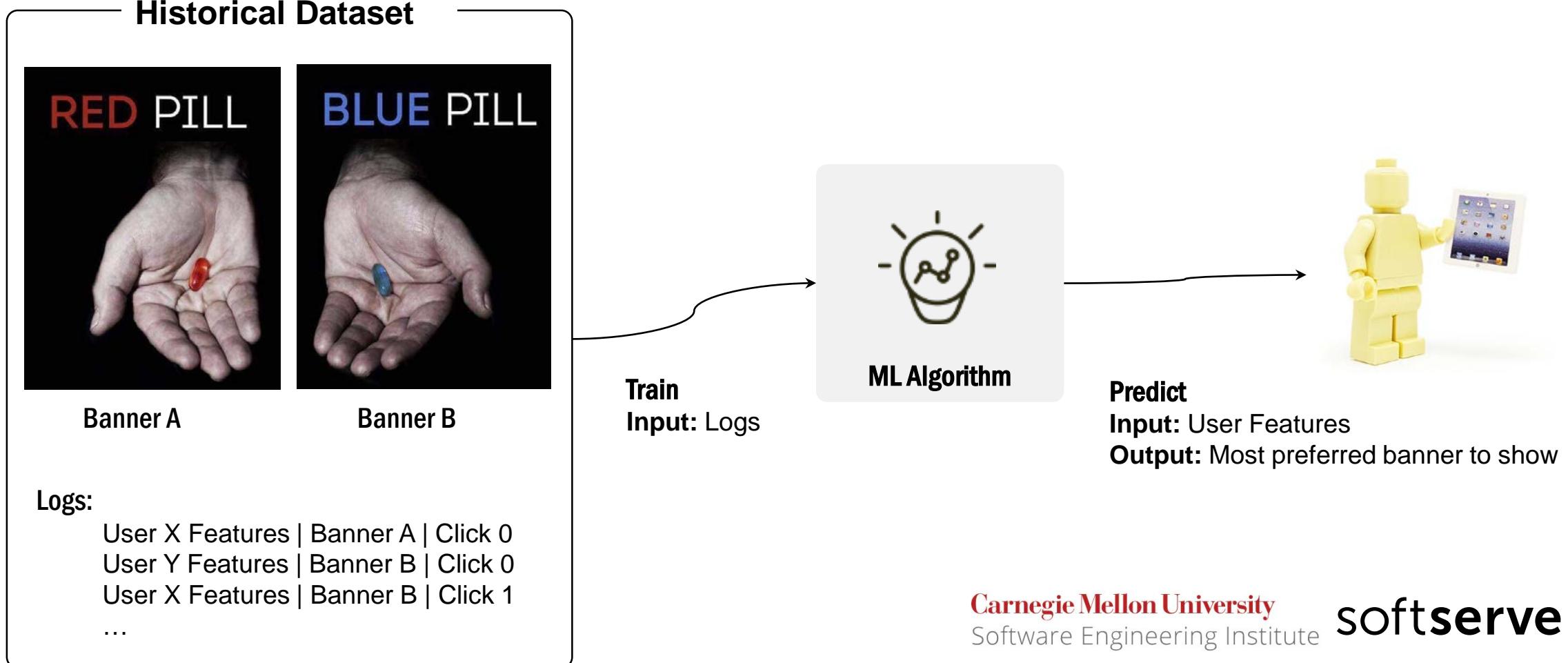


# ITERATION 1:

What type of learning best fits a given use case?

Select from: **supervised** or **unsupervised**

# ITERATION 1: Supervised or Unsupervised Learning?





# MACHINE LEARNING CARDS

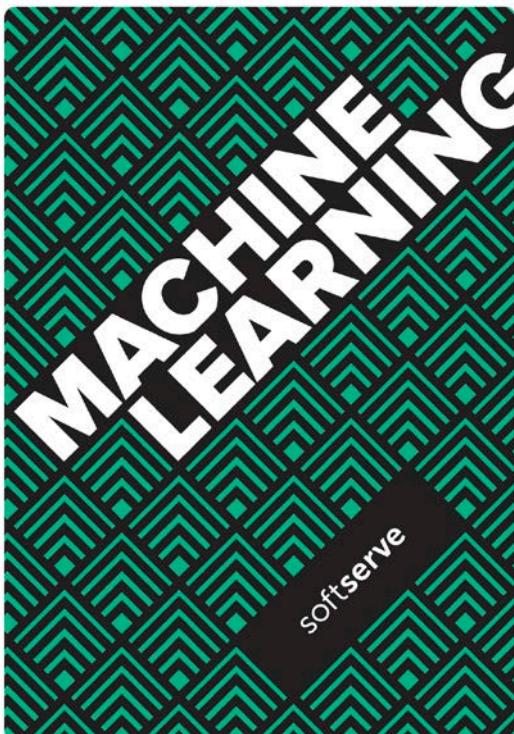
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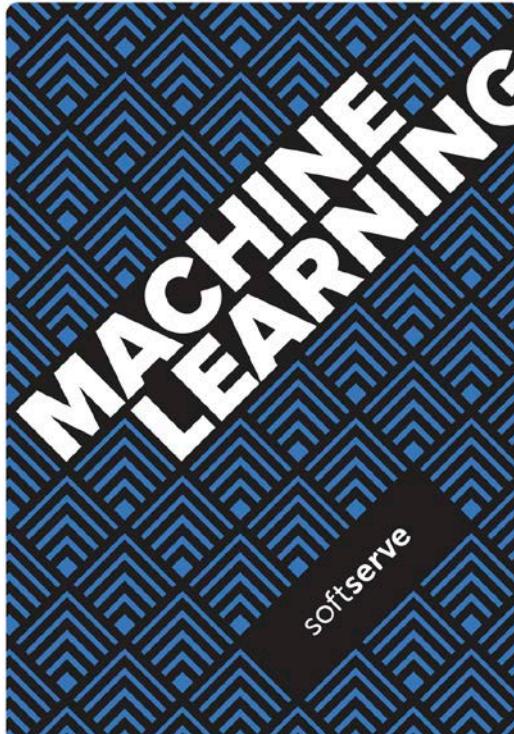
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# MACHINE LEARNING CARDS

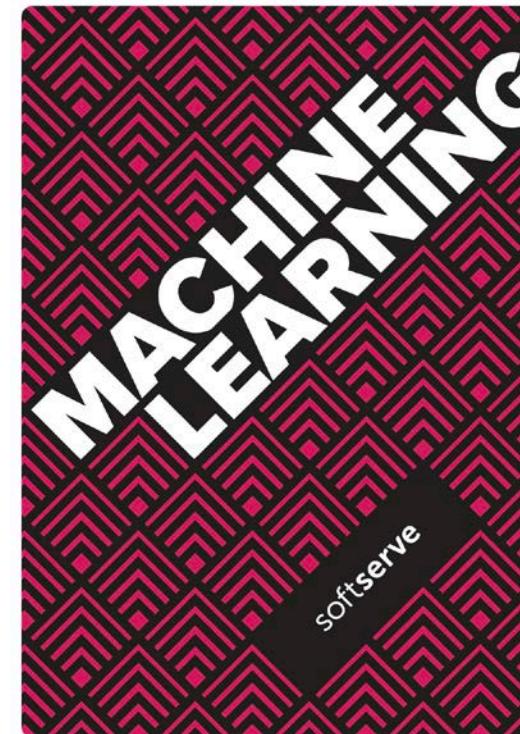
**ITERATION 2:**  
PROBLEM TYPE

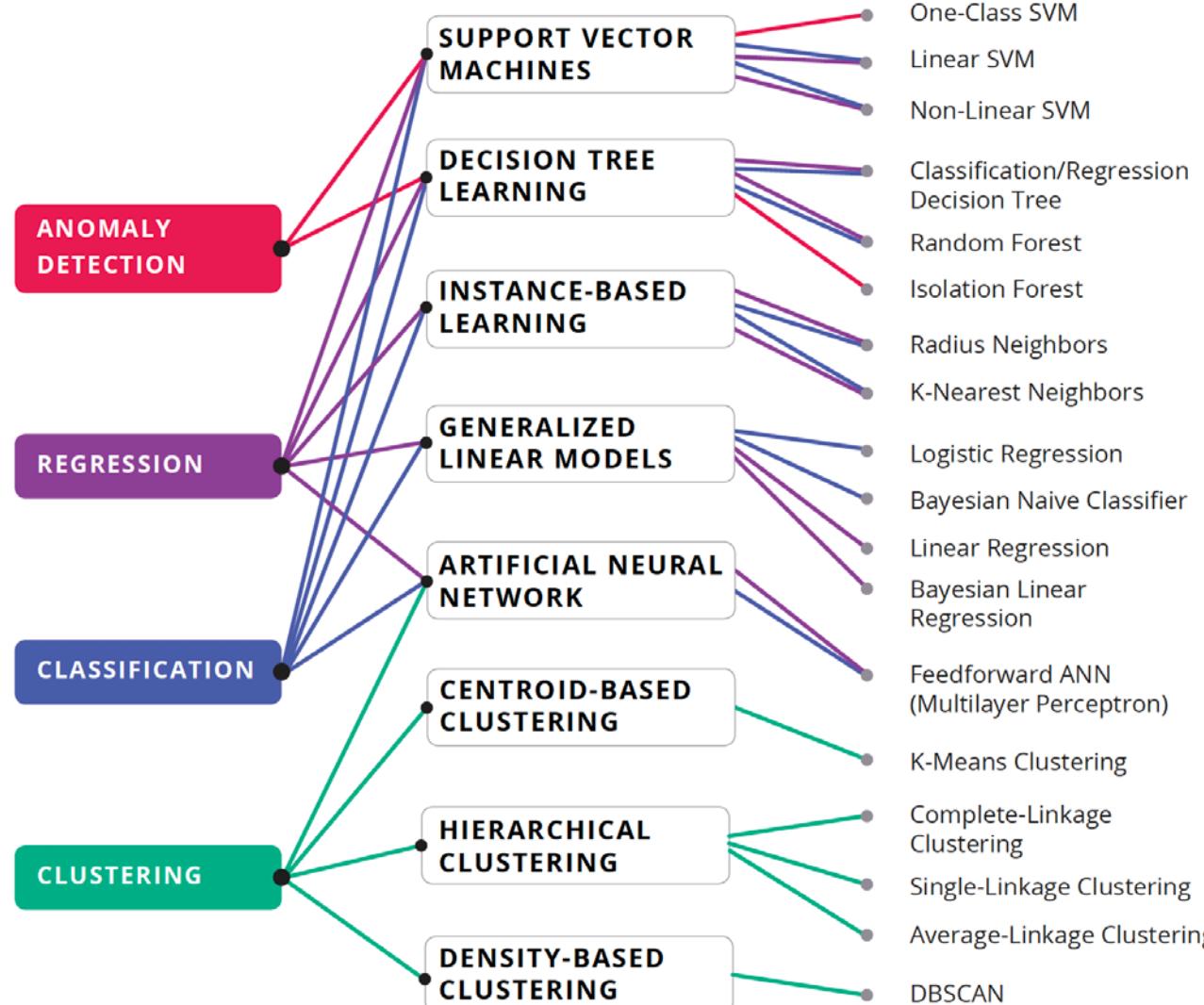
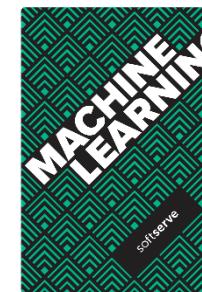


**ITERATION 3a:**  
ALGORITHM FAMILY

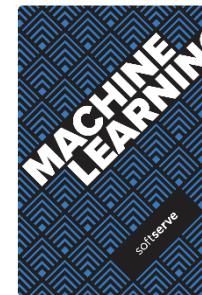


**ITERATION 3b:**  
ML ALGORITHM

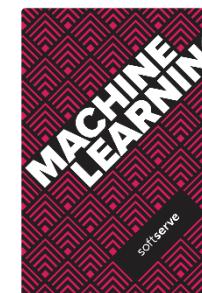


**PROBLEM****ALGORITHM FAMILY****ALGORITHM****Legend:**

- Problem cards



- Algorithm Family cards



- Algorithm cards

# PROBLEM TYPES



# CLASSIFICATION

## Key Highlights:

- Identifies which category an object belongs to
- Supervised learning problem

## Examples:

- Detect fraudulent transactions (one-class)
- Categorize emails by spam or not spam (binary)
- Categorize articles based on their topic (multi-class)
- Detect objects on the image (multi-label)



# REGRESSION

## Key Highlights:

- Predict a continuous value associated with an object
- Supervised learning problem

## Examples:

- Predict stock prices from market data
- Score a credit application based on historical data
- Estimate demand for a given product



# CLUSTERING

## Key Highlights:

- Group similar objects into clusters
- Unsupervised learning problem

## Examples:

- Discover audiences to target on social networks
- Group checking data based on GEO-proximity
- Detect common topics in corporate knowledge base



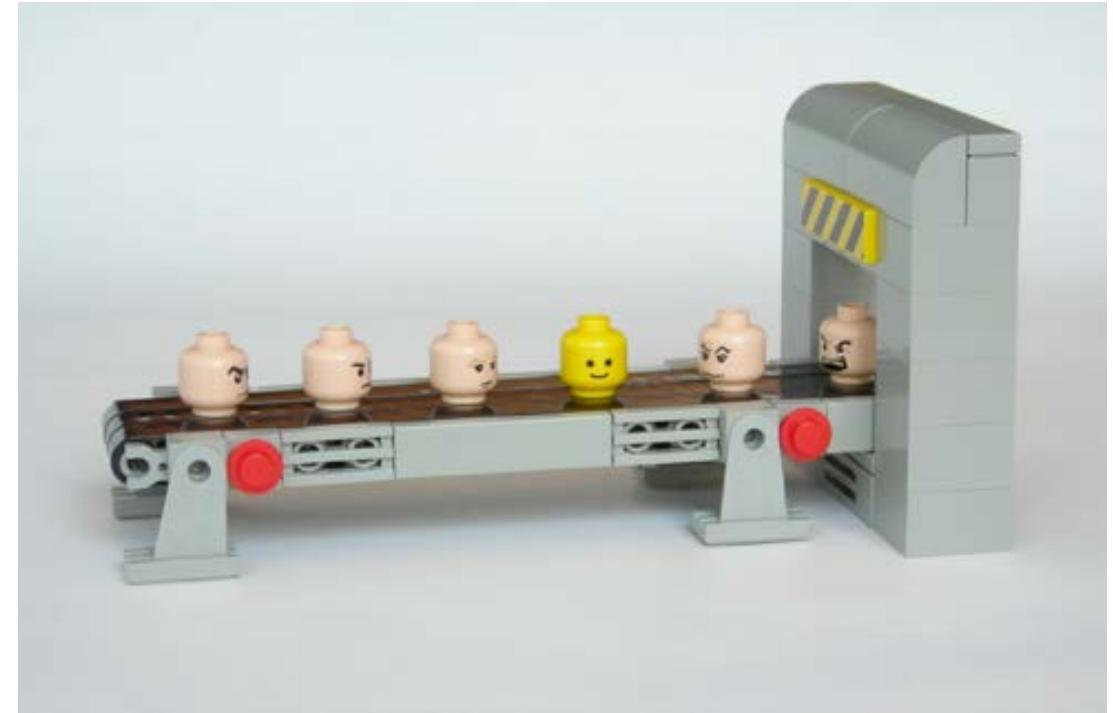
# ANOMALY DETECTION

## Key Highlights:

- Identify observations that do not conform to an expected pattern
- Addresses both supervised and unsupervised learning

## Examples:

- Identify fraudulent transactions or abnormal customer behavior
- In manufacturing, detect physical parts that are likely to fail in the near future



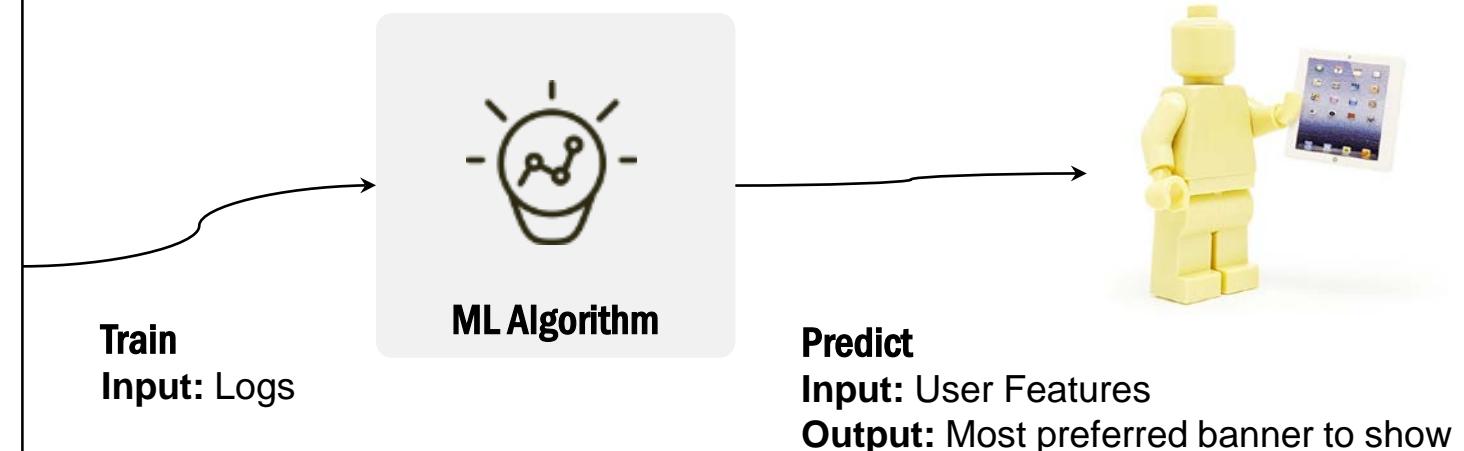
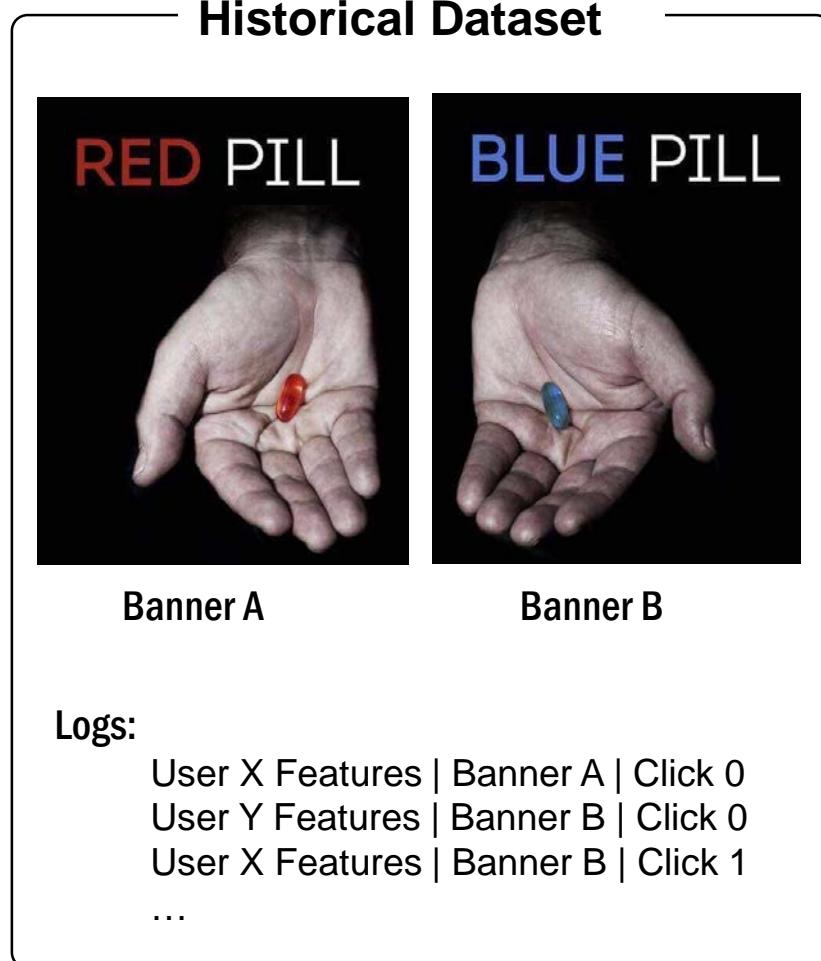
## ITERATION 2:

What type of problem best fits a given use case?

Select problem card from: classification, regression,  
clustering or anomaly detection

# ITERATION 2:

## What type of problem?



# FAMILIES AND ALGORITHMS



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# CLASSIFICATION FAMILIES

## Artificial Neural Network

ALGORITHM FAMILY

**Description:** ANN is a computational model based on the structure and functions of biological neural networks. It can be used for both classification and regression problems, unsupervised learning. The model works well for complex data and complex non-linear relationships but is computationally expensive.

**Characteristics:**

- ★ ★ Big Data — performance positively correlates with volume, but at the expense of computation time.
- ★ Small Data — the less data available, the better other algorithms will outperform neural networks.
- ★ Imbalanced Data — class imbalance increases the possibility of overfitting, but it can be mitigated by adjusting class weights.
- ★ Results Interpretation — usually difficult to interpret.
- ★★★ Online Learning — can be trained sequentially.
- ★ Ease of Use — requires substantial understanding of the ANN field.

**Algorithms:** Feedforward ANN (Multilayer Perceptron), Recurrent Neural Network, Convolutional Neural Network.

MACHINE LEARNING

## Support Vector Machines

ALGORITHM FAMILY

**Description:** SVMs are supervised learning algorithms which can be used for both classification or regression problems (except OneClassSVM which is unsupervised). Given labeled training data, the algorithms output an optimal hyperplane which categorizes new examples.

**Characteristics:**

- ★ Big Data — computation and memory-intensive while training, data sampling can be used as a workaround.
- ★ Small Data — good accuracy even for small # of observations.
- ★★★ Imbalanced Data — compensates imbalance through class weights, works fine out of the box for moderately imbalanced data.
- ★ Results Interpretation — applicable for regulated fields (i.e. credit scoring).
- ★ Online Learning — most implementations only support batch setting.
- ★ Ease of Use — moderate number of parameters.

**Implementations:** Linear SVM, Non-Linear SVM, One-Class SVM.

MACHINE LEARNING

## Generalized Linear Models

ALGORITHM FAMILY

**Description:** A class of linear models with a common property that the dependent variable is linearly related to the independent variables via a specified link function. GLMs were proposed as a way of unifying various approaches.

**Characteristics:**

- Data — there are a lot of implementations, that include iterative approaches, equation systems.
- Data — overfitting resistance due to statistically significant dependencies on balanced Data — poor, can be handled by balance compensations techniques, e.g. bootstrapping.
- Results Interpretation — results drivers of the model.
- Learning — most implementation is sequential setting.
- Ease of Use — models tuning is user-friendly.

**Algorithms:** Logistic Regression, Bayesian Naive Bayes, Bayesian Linear Regression.

MACHINE LEARNING

## Decision Tree Learning

ALGORITHM FAMILY

**Description:** Decision Tree Learning uses a decision tree structure to go from observations about an item to conclusions about the item's target value. It is one of the most interpretable families of machine learning algorithms. This approach can be used for both classification or regression problems.

**Characteristics:**

- Data — generally, the application of this algorithm to large data is not feasible due to memory and prediction restrictions.
- Data — good accuracy, even for a small number of observations.
- Imbalanced Data — more robust for data with imbalanced classes and is efficient for multiclass classification with a small number of features.
- Results Interpretation — transparent inference; process, without the possibility of getting explanation rules.
- Learning — can be trained sequentially.
- Ease of Use — models tuning is user-friendly.

**Algorithms:** Classification/Regression Decision Tree, Random Forest, Isolation Forest.

MACHINE LEARNING

## Instance-Based Learning

ALGORITHM FAMILY

**Description:** Instance-Based Learning (sometimes called nearest neighbor learning) is a family of learning algorithms that performs explicit generalization, compares new instances with instances seen in training and stored in memory. This approach can be used for both classification or regression problems.

**Characteristics:**

- Data — generally, the application of this algorithm to large data is not feasible due to memory and prediction restrictions.
- Data — good accuracy, even for a small number of observations.
- Imbalanced Data — more robust for data with imbalanced classes and is efficient for multiclass classification with a small number of features.
- Results Interpretation — transparent inference; process, without the possibility of getting explanation rules.
- Learning — can be trained sequentially.
- Ease of Use — models tuning is user-friendly.

**Algorithms:** K-Nearest Neighbors, Radius Neighbors.

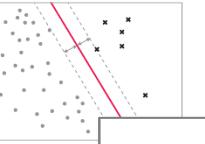
MACHINE LEARNING

# CLASSIFICATION ALGORITHMS

**Linear SVM**

ALGORITHM

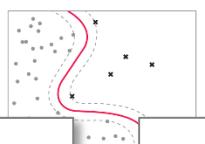
Description: An SVM algorithm with a linear kernel.



**Non-Linear SVM**

SUPPORT VECTOR MACHINES | ALGORITHM

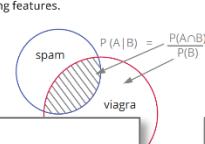
Description: An SVM algorithm with a non-linear kernel like Gaussian (e.g. RBF).



**Bayesian Naive Classifier**

GENERALIZED LINEAR MODELS | ALGORITHM

Description: A simple probabilistic classifier based on Bayes' Theorem with an assumption of strong independence (naïve) among features.

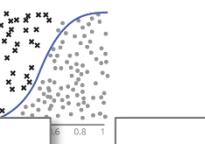


$$P(A|B) = \frac{P(A \cap B)}{P(B)} = \frac{P(B|A)P(A)}{P(B)}$$

**Logistic Regression**

GENERALIZED LINEAR MODELS | ALGORITHM

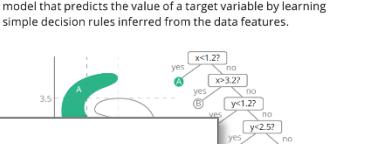
Description: A powerful tool for two-class and multiclass classification. As a linear regression, it is fast and simple.



**Classification/Regression Trees**

DECISION TREE LEARNING | ALGORITHM

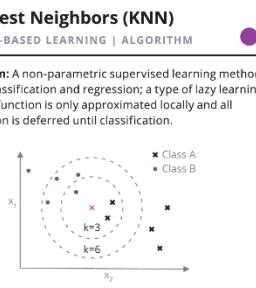
Description: A non-parametric supervised learning method used for classification and regression. The goal is to create a model that predicts the value of a target variable by learning simple decision rules inferred from the data features.



**K-Nearest Neighbors (KNN)**

INSTANCE-BASED LEARNING | ALGORITHM

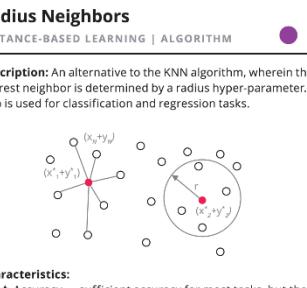
Description: A non-parametric supervised learning method used for classification and regression; a type of lazy learning, where the function is only approximated locally and all computation is deferred until classification.



**Radius Neighbors**

INSTANCE-BASED LEARNING | ALGORITHM

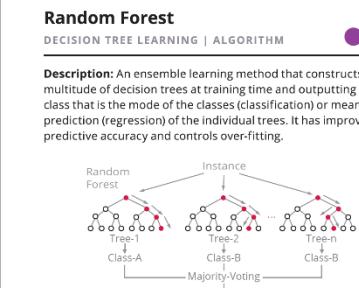
Description: An alternative to the KNN algorithm, wherein the nearest neighbor is determined by a radius hyper-parameter. Also is used for classification and regression tasks.



**Random Forest**

DECISION TREE LEARNING | ALGORITHM

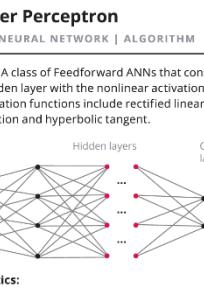
Description: An ensemble learning method that constructs a multitude of decision trees at training time and outputting the class that is the mode of the classes (classification) or mean prediction (regression) of the individual trees. It has improved predictive accuracy and controls over-fitting.



**Multilayer Perceptron**

ARTIFICIAL NEURAL NETWORK | ALGORITHM

Description: A class of Feedforward ANNs that consists of at least one hidden layer with the nonlinear activation function. Popular activation functions include rectified linear unit (ReLU), sigmoid function and hyperbolic tangent.



**Tips:**

- ✓ Great performance in high-dim
- ✓ Works well in case when # of features
- ✓ Margins maximization provides

**Implementations:** R, Python (scikit-learn), Spark (mllib), Azure.

MACHINE LEARNING

**Characteristics:**

- ★ Accuracy — depends on dataset size
- ★ Training Speed — linear depending on dataset size
- ★★ Prediction Speed — depends on number of features
- ★★ Overfitting Resistance — depends on number of hyperparameters
- ★ Probabilistic Interpretation — provides

**Tips:**

- ✓ Great performance in high-dim
- ✓ Works well in case when # of features
- ✓ Margins maximization provides

**Implementations:** R, Python (scikit-learn), Spark (mllib), Azure.

MACHINE LEARNING

**Characteristics:**

- ★★ Accuracy — depends on dataset size
- ★★ Training Speed — linear depending on dataset size
- ★★ Prediction Speed — full training set processing is required
- ★★ Overfitting Resistance — with an increase of k nearest training objects, the probability of overfitting decreases
- ★★ Probabilistic Interpretation — naturally determined by the inference process

**Tips:**

- ✓ One of the simplest machine learning algorithms
- ✓ Good choice for low dimensional space

**Implementations:** R, Python (scikit-learn).

MACHINE LEARNING

**Characteristics:**

- ★★ Accuracy — sufficient accuracy for most tasks, but there is a tradeoff between accuracy vs avoiding overfitting
- ★★ Training Speed — training time is high on large datasets
- ★★ Prediction Speed — full training set processing is required
- ★★ Overfitting Resistance — with an increase of radius the probability of overfitting decreases
- ★★ Probabilistic Interpretation — naturally determined by the inference process

**Tips:**

- ✓ One of the simplest machine learning algorithms
- ✓ Good choice for data that isn't sampled uniformly
- ✓ For high-dimensional spaces, this method is less effective due to so-called "curse of dimensionality"

**Implementations:** R, Python (scikit-learn).

MACHINE LEARNING

**Characteristics:**

- ★★★ Accuracy — due to bootstrap aggregation of independent trees
- ★★★ Training Speed — depends on model complexity, but it can be parallelized
- ★★★ Prediction Speed — depends on model complexity but it can be improved due to independent trees
- ★★★ Overfitting Resistance — complexity doesn't lead to overfitting
- ★★★ Probabilistic Interpretation — can be extracted

**Tips:**

- ✓ Naturally works with both categorical and numerical data
- ✓ High accuracy without extensive tuning

**Implementations:** R, Python (scikit-learn), Spark (mllib), Azure.

MACHINE LEARNING

**Characteristics:**

- ★★★★ Accuracy — works well for both linear and nonlinear dependencies
- ★★★★ Training Speed — depends heavily on model complexity and on training dataset size
- ★★★★ Prediction Speed — depends on # of model features, scales well
- ★★★★ Overfitting Resistance — requires big training set and regularization
- ★★★★ Probabilistic Interpretation — thanks to the softmax activation

**Tips:**

- ✓ Good performance for high dimensional space
- ✓ Works well with numerical and categorical data

**Implementations:** R, Python (scikit-learn), Spark (mllib), Azure.

MACHINE LEARNING

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# DECISION DRIVERS



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# FAMILY DRIVERS

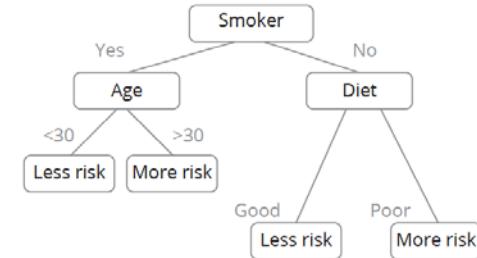
- **Big Data** – scalability and ability to leverage from new data
- Small Data – ability to learn from a few examples
- **Imbalanced Data** – ability to distinguish rare events
- Results Interpretation – human-friendly results
- Online Learning – ability to continuously train from new data
- **Ease of Use** – number of parameters to manually tune

## Decision Tree Learning

ALGORITHM FAMILY



**Description:** Decision Tree Learning uses a decision tree structure to go from observations about an item to conclusions about the item's target value. It is one of the most interpretable families of machine learning algorithms. This approach can be used for both classification or regression problems.



### Characteristics:

- ★★ Big Data — interpretability is getting worse on large datasets
- ★★ Small Data — sufficient generalization even for very small dataset, but can lead to overfitting
- ★★ Imbalanced Data — can be handled by stratified bootstrap technique
- ★★★ Results Interpretation — represented by a set of decision rules
- ★★★ Online Learning — can be trained sequentially
- ★★★ Ease of Use — models tuning is user-friendly

**Algorithms:** Classification/Regression Decision Tree, Random Forest, Isolation Forest.

MACHINE LEARNING

# ALGORITHM DRIVERS

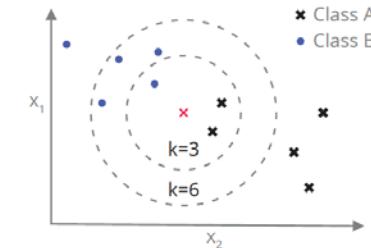
- **Accuracy** – ability to solve complex problems
- **Training Speed** – training runtime performance
- **Prediction Speed** – production runtime performance
- Overfitting Resistance – ability to generalize to new data
- Probabilistic Interpretation – return results as probabilities

## K-Nearest Neighbors (KNN)

INSTANCE-BASED LEARNING | ALGORITHM



**Description:** A non-parametric supervised learning method used for classification and regression; a type of lazy learning, where the function is only approximated locally and all computation is deferred until classification.



### Characteristics:

- ★★ Accuracy — sufficient accuracy for most tasks, but there is a tradeoff between accuracy vs avoiding overfitting
- ★★ Training Speed — training time is high on large datasets
- ★ Prediction Speed — full training set processing is required
- ★★ Overfitting Resistance — with an increase of k nearest training objects, the probability of overfitting decreases
- ★★★ Probabilistic Interpretation — naturally determined by the inference process

### Tips:

- ✓ One of the simplest machine learning algorithms
- ✓ Good choice for low dimensional space

**Implementations:** R, Python (scikit-learn).

MACHINE LEARNING

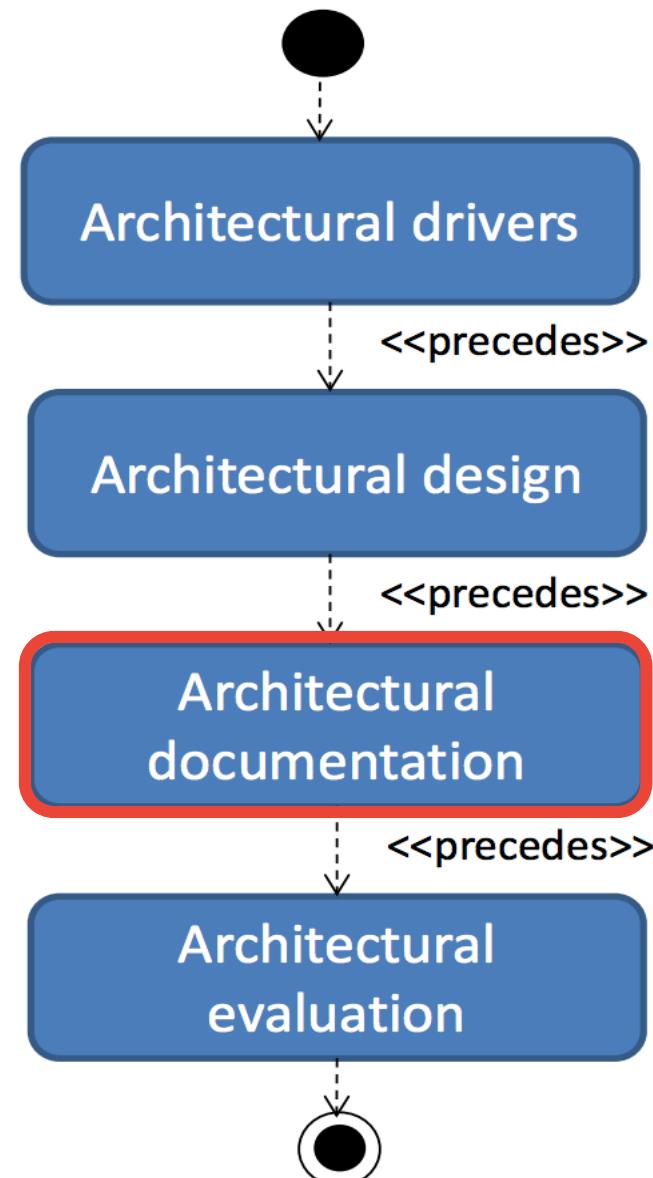
## ITERATION 3:

Select a family and an algorithm card that would best fit a given use case

Family Key Drivers: **Big Data, Imbalanced Data, Ease of Use**

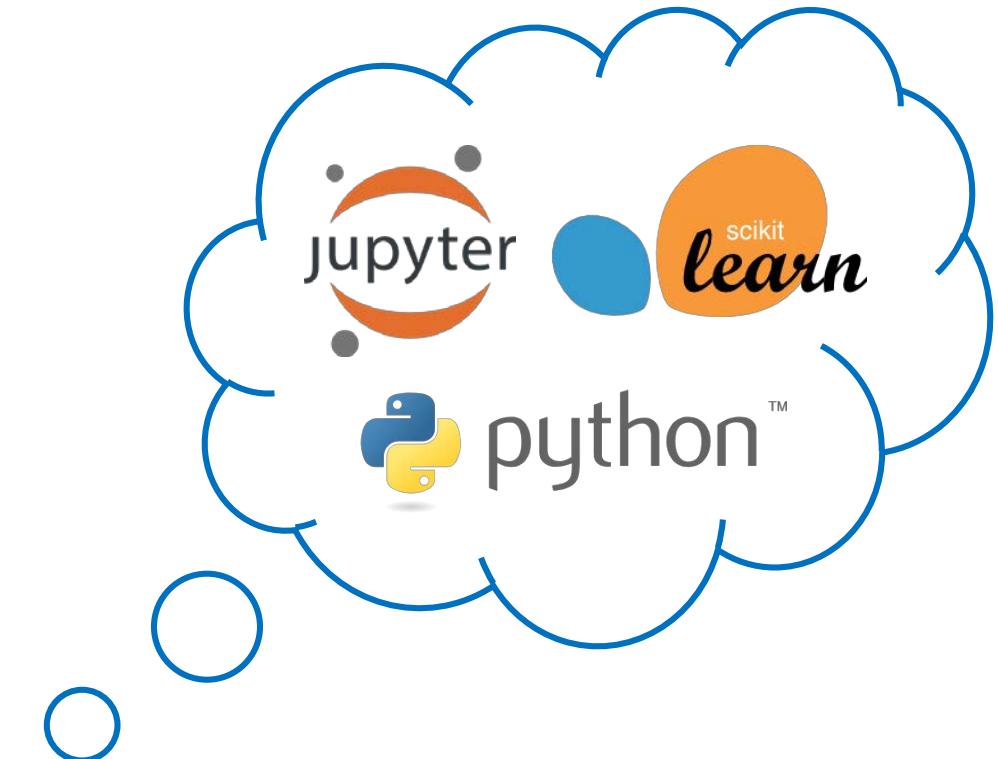
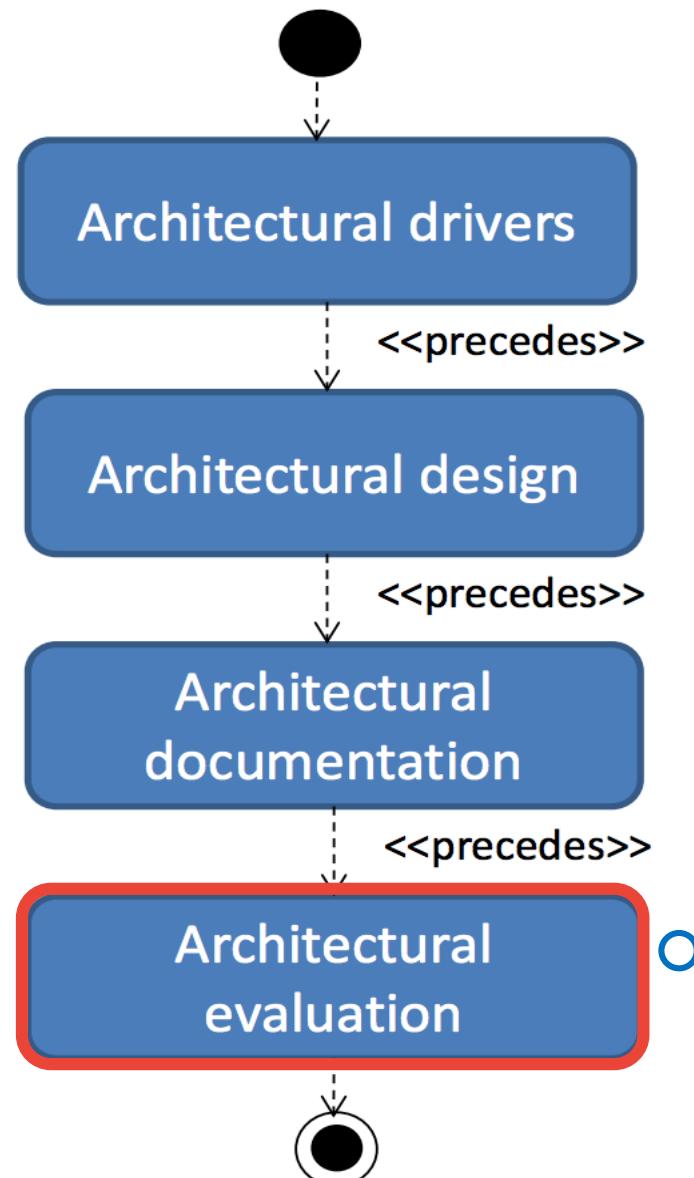
Algorithm Key Drivers: **Accuracy, Training and Prediction Speed**

# DESIGN PROCESS



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# DESIGN PROCESS



# PROTOTYPING AND EVALUATION SESSION

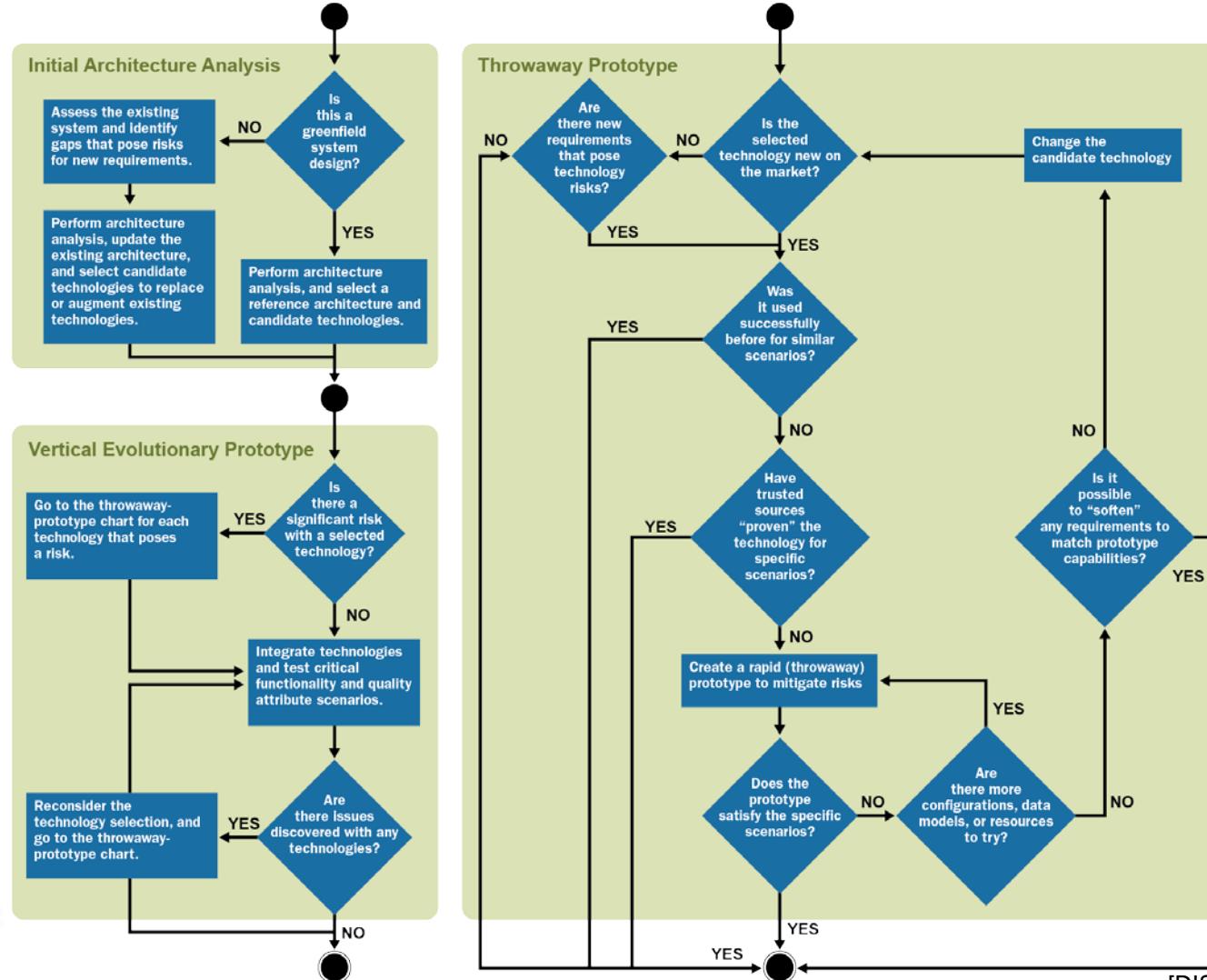


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# PROTOTYPING FOR EVALUATION



# RESULTS SUMMARY

Algorithm name	Training Time	Prediction Time	Tuning Time	Initial Accuracy	Final Accuracy
Random Forest	2.61	0.47	94.44	81.61%	83.05%
KNeighbors	0.41	44.29	84.27	80.57%	83.05%
Logistic Regression	0.12	0.05	45.94	82.93%	82.93%
MLP	0.80	0.08	164.04	66.25%	82.90%
SVM	177.78	54.87	973.73	82.83%	82.83%
Linear SVM	5.93	0.04	82.91	82.69%	82.69%
Decision Trees	0.03	0.005	52.97	73.16%	82.36%
Naive Bayes	0.02	0.01	0	78.46%	78.46%

# KEY TAKEAWAYS



- Machine Learning solution design is an iterative process
- ADD principles help make ML design decisions in a systematic way
- ML Cards aim to select candidate algorithms from a wide variety of alternatives
- Prototyping is necessary to validate design decisions

QUESTIONS?  
WE'VE GOT THE  
ANSWERS.

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