



From data science to data stories:

Integrating predictive analytics into

R&D and Manufacturing

# AI is ready for us

## October 2017 – AlphaGo Zero beats AlphaGo in 3 days

Reinforcement learning algorithms and blank slate learning allow AlphaGo Zero to learn optimal strategies of Go

## December 2017 – AlphaGo Zero learns chess in a day and becomes Alpha Zero

AlphaZero beats Stockfish – the state of the art player with 64:36, running 80K positions per second vs. 7 Mln positions per second

## January 2018 – AI systems win from humans in SQuAD

Alibaba' and Microsoft' AI systems won over humans in the listening comprehension test

Sources: <https://en.chessbase.com/post/the-future-is-here-alphazero-learns-chess>,

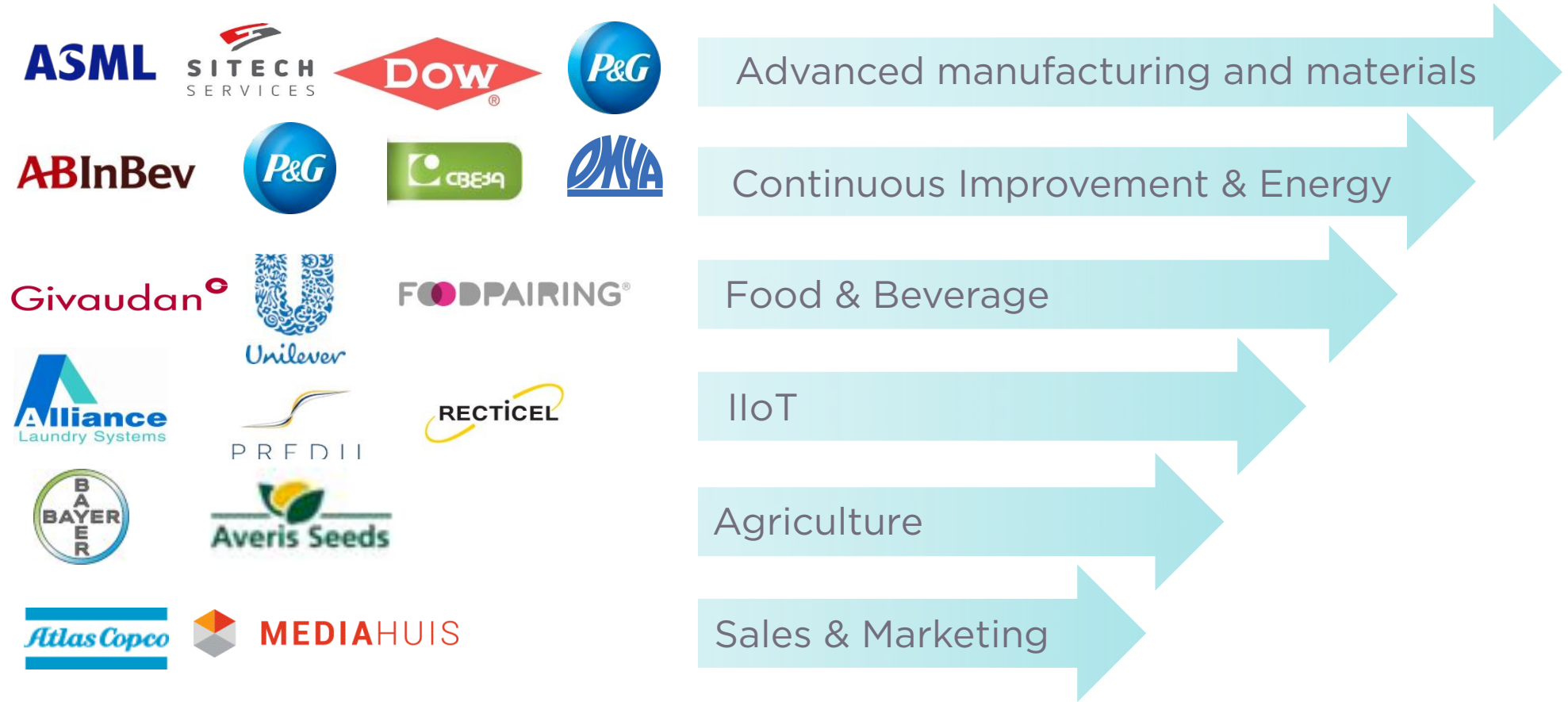


**If you can measure it,  
you can understand it.**

**If you can understand  
it, you can alter it.**

*Katherine Neville*

# Our technology is shaped by the real world



# CHALLENGES

Almost any business in any industry struggles with four challenges

1. How are all parts of my complex process related to each other?

2. What impacts the outcomes?

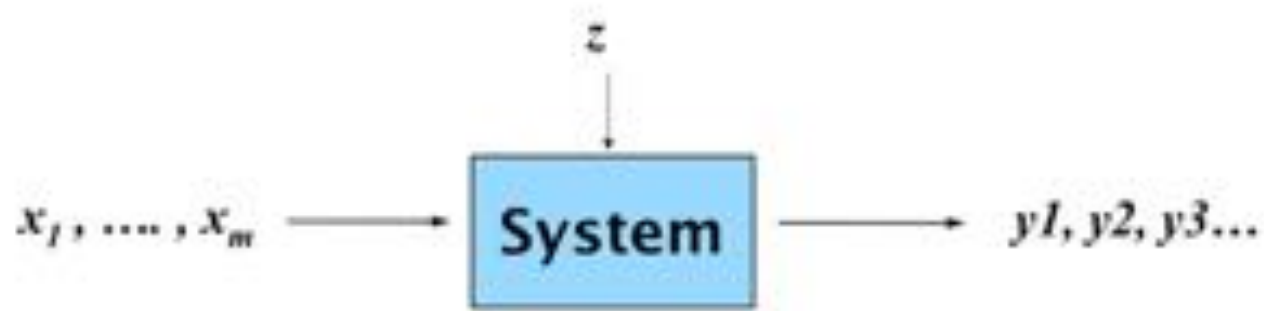
3. What should I change and by how much to achieve desired outcomes?

4. What are exceptions to the rules?



# DATA-DRIVEN

The goal is to understand the system to alter its behavior



$$y = f(x_{i1}, \dots, x_{ik})$$

	Input variables				Responses		
	$x_1$	$x_2$	...	$x_d$	$y_1$	...	$y_r$
Data Records	•	•		•	•		•
	•			•	•		•
	•	•		•	•		•
	•		...	•	•		•
	•	•		•	•		•
...	...		...	...	...		...







**Samuel Karlin**

***"The purpose of models is not to fit the data but to sharpen the questions."***

**FUTURE**

# Augmented Analytics for Augmented Intelligence

**Automating insight generation based on advanced machine learning and artificial intelligence.**

**Gartner** | *“Next Wave of Analytics Disruption”*





Everything around us needs to be re-designed. Now

- 1. 95% of data is underutilized**
- 2. Access to great data scientists is limited**
- 3. Domain experts make final decisions**



## Put domain experts central and communicate your data analytics outcomes as actionable data stories



Predictive analytics solutions have a future in a company only when they are understood and internalized by domain experts and decision takers.

DataStories software brings advanced analytics tools in the hands of domain experts and delivers strategic business insights the same day.

Only when translated into stories, recommendations have a chance to propagate through the company and be successfully deployed.

DataStories offer a range of fully automated machine learning algorithms and predictive analytics workflows, translated into simple interactive data stories - reports with immediately actionable recommendations.



data**stories**

is advanced predictive  
analytics partner  
for industrial businesses  
with complex R&D and  
manufacturing processes  
generating lots of data



# ONE MISSION

**EMPOWERING PEOPLE TO USE  
PREDICTIVE DATA ANALYTICS IN THEIR  
DAY-TO-DAY WORK  
VIA SIMPLE STORIES.**



# Focus on Research & Development and Research & Innovation Departments in Life Sciences:

## R&D and R&I

- Performance Chemicals
- Advanced Materials R&D
- Life Sciences - Food & Flavor R&D (FMCG)
- Advanced Machinery
- Life Sciences – beauty
- Life Sciences – pharma
- Life Sciences – prevention & longevity
- Life Sciences – Agriculture

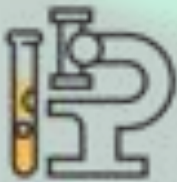
## Manufacturing

## Sales & marketing

## Fashion

## Financial

**R&D**



**Customer  
Intelligence**



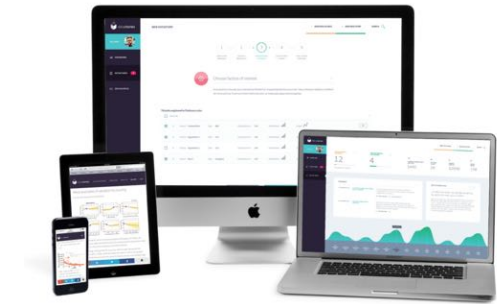
**Continuous  
Improvement**



datastories

# PRODUCTS

## Cloud, Standalone or Enterprise Hosted solutions and Premium Training & Support



- ✓ Browser-based self-service analytics for non-data scientists
- ✓ Interactive narrative of what matters in your data
- ✓ Fully automated analysis workflow
- ✓ Export predictive models to Excel or C/C++
- ✓ Automatic export to Powerpoint



- ✓ Automated analytics toolbox for Matlab® users
- ✓ 4-step automatable analysis workflow with complete GUI support
- ✓ Automatic scaling
- ✓ Automatic handling of categorical variables
- ✓ Robust predictive models with local error bounds



- ✓ Full option for consultants, data scientists and engineers
- ✓ Interactive narrative of what matters in your data
- ✓ Fully automated analysis workflows
- ✓ Best in class algorithms for variable selection and ML for regression



- ✓ Custom big data consulting by award-winning data scientists
- ✓ Custom data preparation & wrangling
- ✓ Model-guided experimental design
- ✓ Custom engine development



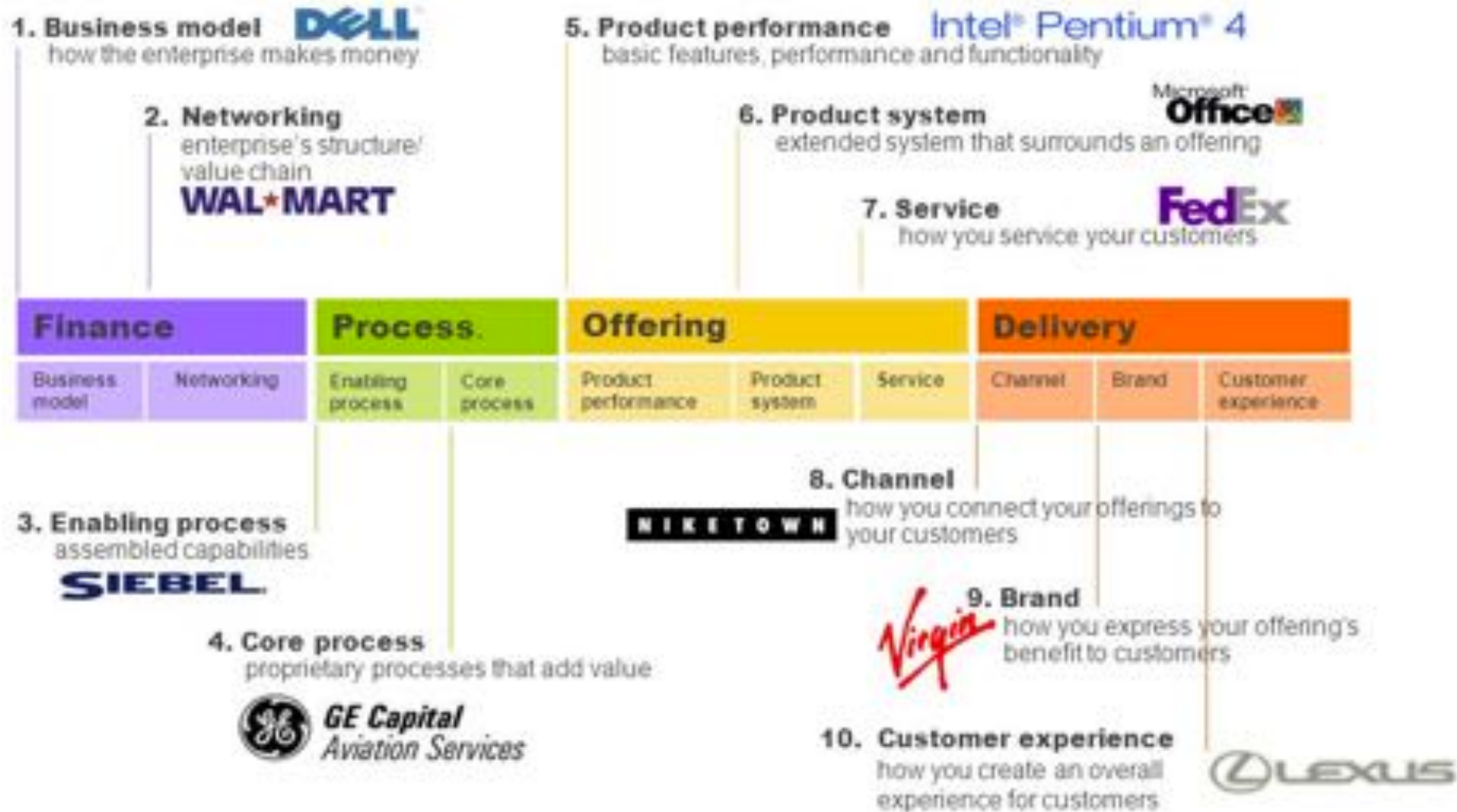


## Cloud, Standalone or Enterprise Hosted solutions and Premium Training & Support

- Speed of algorithm development
- Flexibility with integrations
- Seamless expansion to HPC
- Code protection
- Massive scalability for different product forms
  - platform, toolbox for MATLAB, API



# 10 types of Innovation: Move Beyond Products to Win



# Research & Development

## DESIGN EXPERIMENTS

Plan and collect the data by optimally varying compositions and process conditions

## OPTIMIZE TARGETS

Optimize models to get optimal settings for optimal potentially competing targets

## DEPLOY MODELS

Robust Prediction Profilers and interactive sensitivity analysis identify future experiments

## ANALYZE MODELS

Robust ensemble-based methods help identify driving factors and build robust predictions

## ASSEMBLE DATA SOURCES

Organize the data intelligently, think of labelling, ontologies, continuity. Add new experimental data

## ADD NUMERIC DESCRIPTORS

Critically important step to augment the composition data with computable numerical descriptors

## VISUALIZE & RUN STATS

Explore the experimental data visually, identify visible problems, errors, data density, duplicates, etc

## MODELING

The goal of modeling in the augmented space is to identify descriptors and conditions that drive performance





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### BUILD MODELS

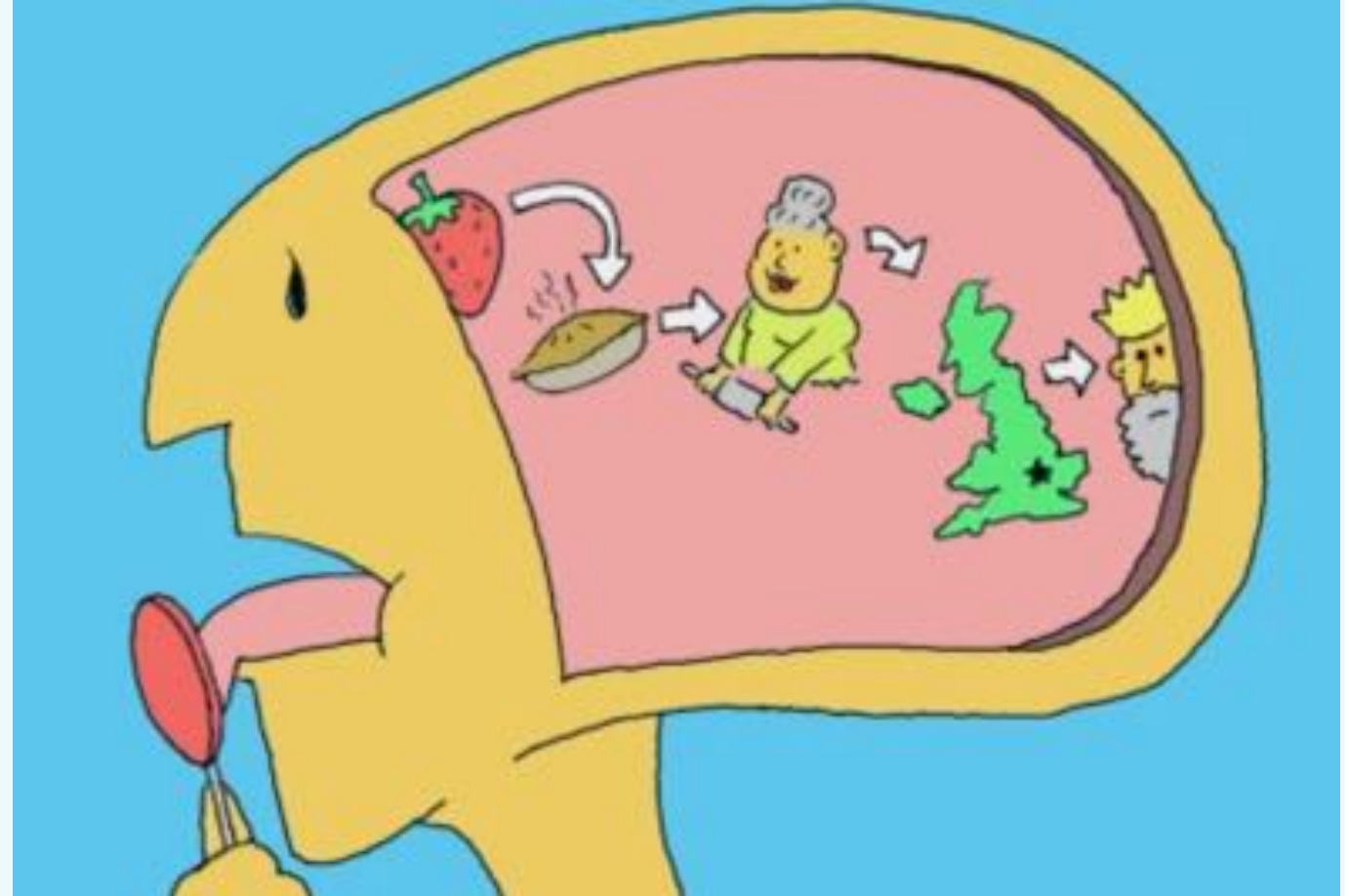
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# CUSTOMER INTELLIGENCE

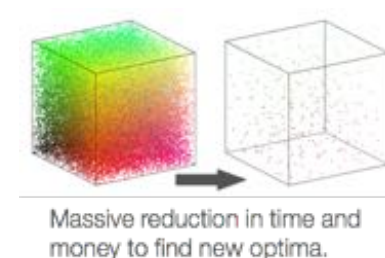
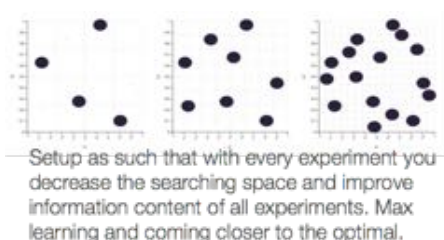
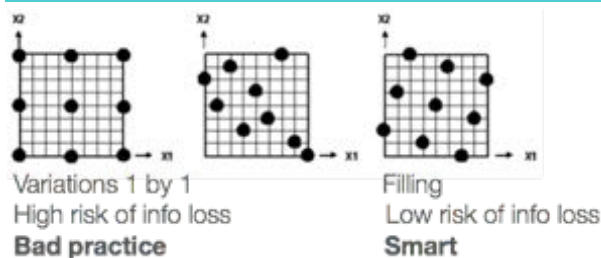
Unique expertise and technology for discovering contextual features driving liking from customer reviews

DataStories Feature Engineering tools and technology help handle and interpret massive design spaces of sparse data (e.g. hundreds of thousands of users, tens of thousands of product and review features with lots of missing data)

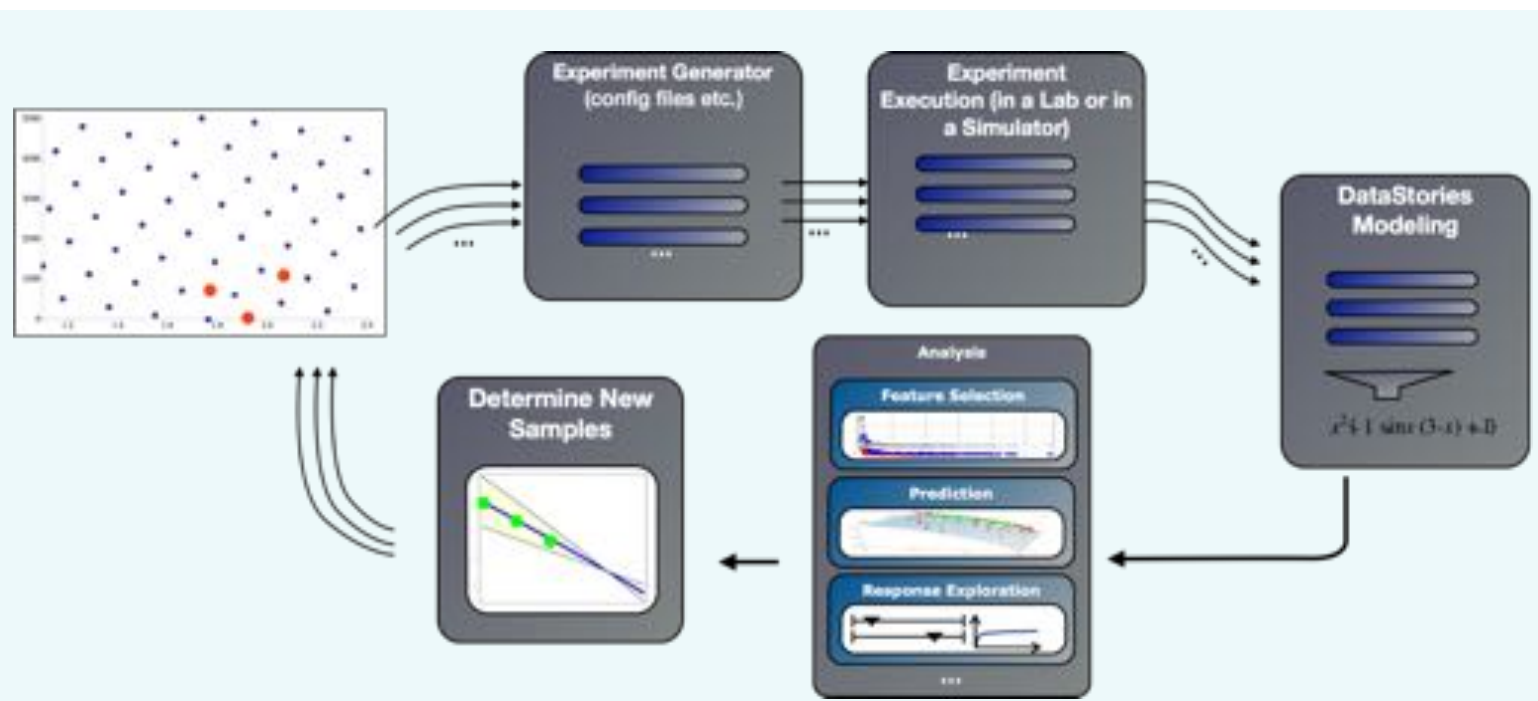


# SMART DOE

## Smart Design of Experiments Workflow for Model-guided product optimization



Robust and field-tested DOE workflows help explore huge spaces of product/compound features (chemical, sensory, contextual and perception descriptors) and guarantee systematic innovation.





# COMPOUND DESIGN

## DataStories' Predictive AI algorithms dramatically accelerate compound discovery

Make predictions for unknown compounds, products, packaging, services taking into account variability in thousands of descriptors

Understand what drives performance targets

Create and interactively profile robust predictive models using key performance drivers

Scan millions of compounds in-silico and identify optimal solutions to guide product design

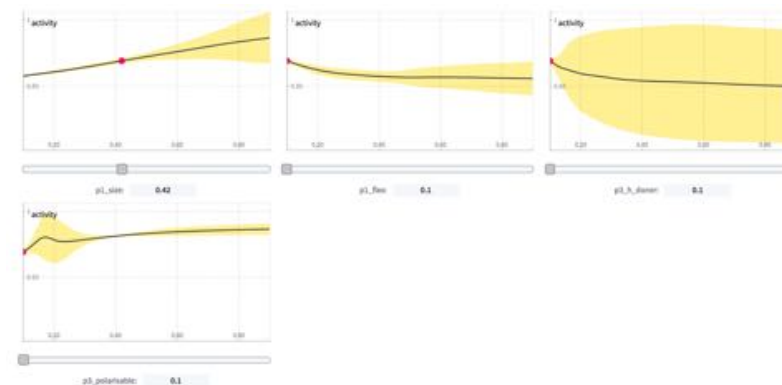
Find suitable descriptors for each product type



Significant reduction in search space and ... everything is numeric now

Name	Structure	bp, °C	spose minima s	descriptors in coats
water	<chem>H2O</chem>	100	1.07	50
methanol	<chem>CO</chem>	65	1.7	33
ethanol	<chem>CCO</chem>	78	1.6	24.3
isopropanol	<chem>CC(C)O</chem>	82	1.6	20.1
1-butanol	<chem>CCCCO</chem>	118	1.6	17.8
formic acid	<chem>C=O</chem>	100	1.73	50
acetic acid	<chem>CC=O</chem>	118	1.6	6.5
formamide	<chem>CC=O</chem>	210	1.73	50
acetone	<chem>CC(C)=O</chem>	56	2.88	20.7
triethylamine (TEA)	<chem>CC(C)N</chem>	69	1.63	7.52
methyl ethyl ketone	<chem>CC(C)C=O</chem>	80	2.78	10.5
ethyl acetate	<chem>CC(=O)CC</chem>	77	1.78	6.02
acetamide	<chem>CC(N)=O</chem>	221	1.92	30.8
N,N-dimethylformamide (DMF)	<chem>CN(C)C=O</chem>	38	3.02	38.3
dimethyl sulfoxide (DMSO)	<chem>CSC(S)=O</chem>	189	3.06	47.2
hexane	<chem>CCCCC</chem>	69	1.6	2.02
benzene	<chem>C1=CC=CC=C1</chem>	80	0	2.29
ethyl ether	<chem>CCOCC</chem>	35	1.8	6.34
methylene chloride	<chem>CN=C</chem>	40	1.6	3.02
carbon tetrachloride	<chem>CCl(Cl)Cl</chem>	77	0	2.24

Partial Solvents Product List



# Manufacturing

# MANUFACTURING INTELLIGENCE

Unique expertise and technology for discovering production performance drivers and optimal setpoints

Handle massive amounts of sensor data and complicated processes (batch, continuous, discrete)

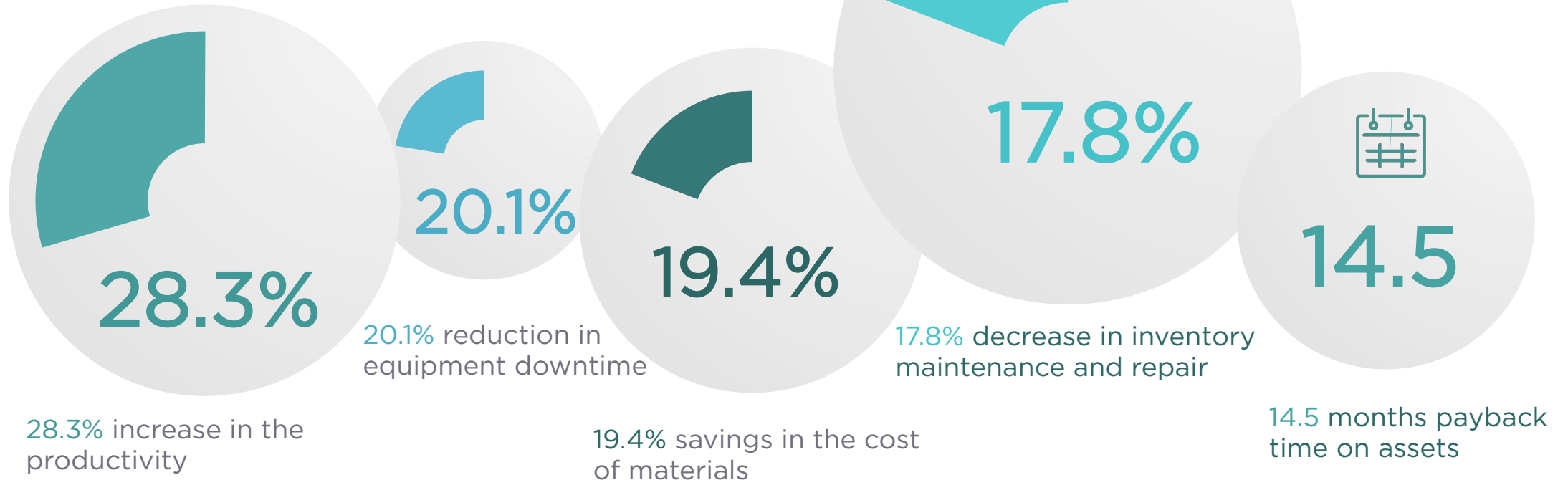
Help discover outcome drivers, and optimize operational target ranges

Quantify process sensitivity towards varying raw material quality, operating teams, recipes





“ According to an A. T. Kearney survey in Industry Week, 558 companies that currently use computerized maintenance management systems exhibited average improvements of

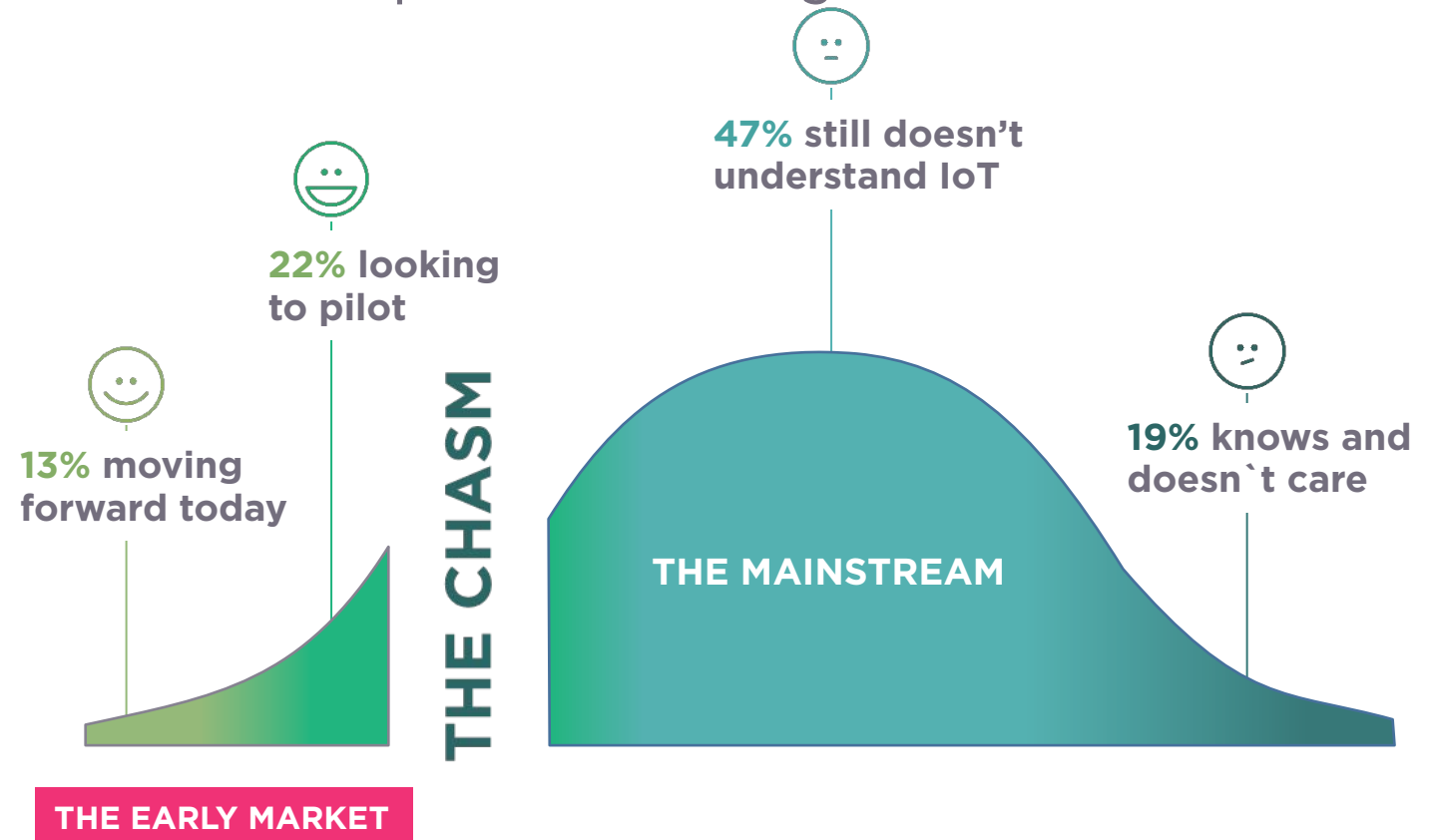


# IoT & Products-as-a-service allow Product Differentiation

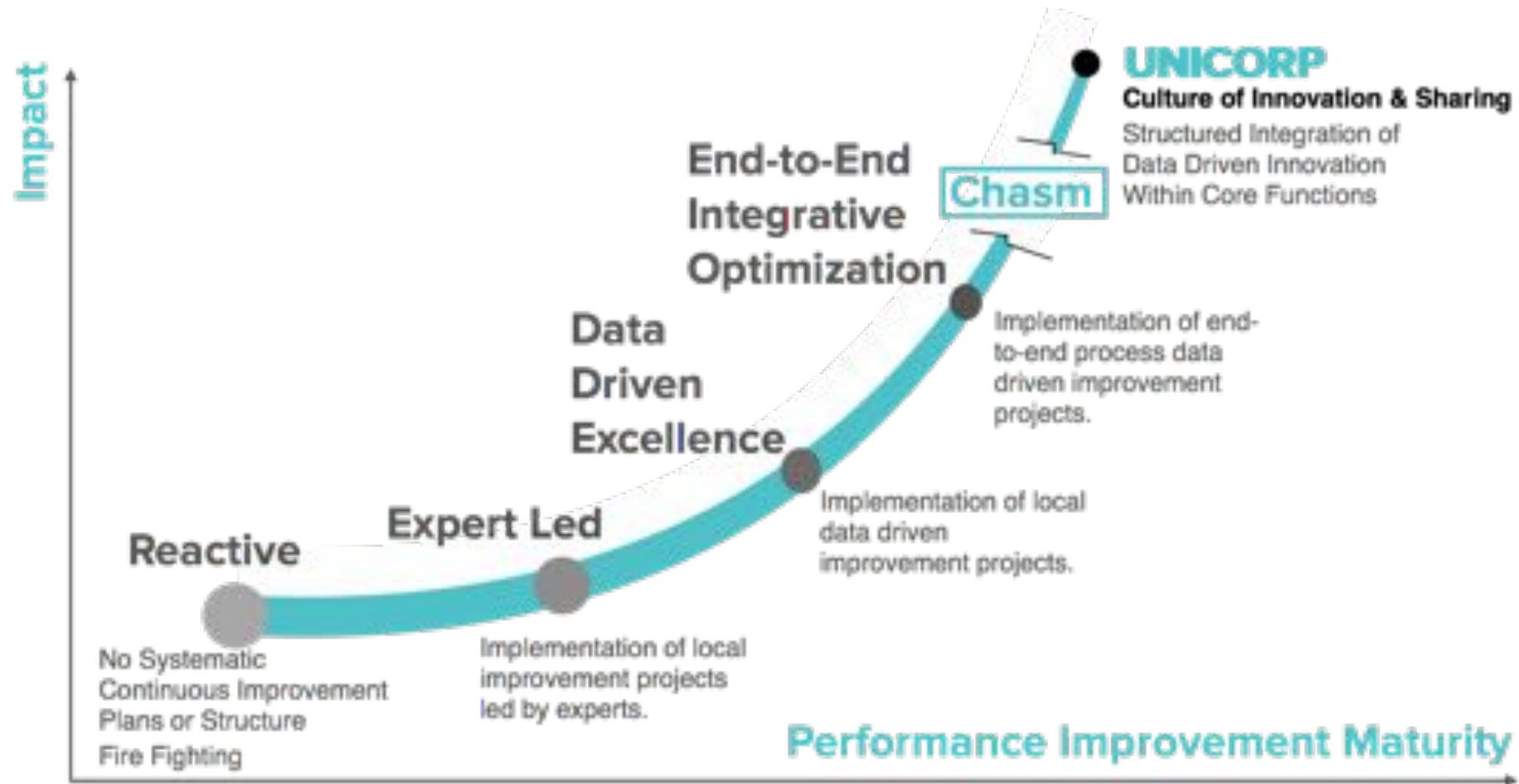
Improved competitiveness, increased **product and service innovation**

- ✓ Possible applications: Repair prevention, Customized service contracts based on usage, advice on how to save water and electricity, Usage reports with advice on improved exploitation will help build customer relationships and possibly target promotions

Crossing the Traditional Chasm for data-driven production management



# Crossing the chasm of data-driven maturity



# Big Data Analytics is the answer, but what is the question?



Predictive and  
Preventive  
maintenance



Demand  
forecasting



Equipment  
utilization





New products R&D



Energy management



Servitization



Process Optimization



Connecting Simulation to Sensor data



Quality Improvement



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