# FEATURE ENGINEERING

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And Other Methods to Prep Lab Data for Integration with Machine Learning Models



Use **digital tools** to change how the ethanol industry collects, maintains, and analyzes data to gain more **accurate insights** in **less time** while utilizing **fewer resources**.

#### **Advanced Data Solutions**

Maximize your now

Flexible data processing, customizable reporting, and advanced analytics

Aimed to help you make the most of the data generated across your plant and reduce the time to actionable insight

**Data Processing and Advanced Analytics** 

#### **Virtual Plant Technology**

Predict your future

Predictive models driven by science and engineering fundamentals

Aimed to help you look to the future and make informed decisions about products and process changes

Dynamic Fermentation Modeling Holistic Process Modeling



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# WHY DO WE NEED STATISTICS

### **Dealing with Uncertainty**



# WHY DO WE NEED STATISTICS

### **Dealing with Uncertainty from Samples**



HPLC Data, Lab Data, Sieve Analysis, Yeast Health, Solids, etc. (anything where you are analyzing samples)

# **OBJECTIVES**

## What is the goal of the talk today?



What can you do for you?



What can I do for you?



### What can AI do for you?



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## **OBJECTIVES**



Data Upload

Data Cleaning and Outlier Analysis

**Process Screening** 

Feature Engineering

Least Square Linear Models (Multiple Features)



Performance Metric Evaluation

Batch Linking

Fit Curve Analysis

Direct/Indirect Feature Analysis

Variability Analysis

Predictor Screening, Partition Modeling



#### Trained/Validated ML Models

Model Evaluation

**Probabilistic Action Items** 

Local Data Analysis

Dynamic Time Warping

# DATA UPLOAD

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# DATA UPLOAD

- Utilizing coding to improve the process Routine reports can be uploaded faster by coding (scripting, macros) to transform raw data into a workable data table.
- Consistency is key Automated data is guaranteed to be consistent and not contain different features, columns, formats, etc.
- Faster Turnaround Time Minimizes time spent uploading and cleaning, meaning more time spent analyzing data and providing insights.



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# DATA CLEANING OUTLIER ANALYSIS

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## **ALWAYS GRAPH YOUR DATA**



These graphs all show the exact same output in terms of R-squared. Are they the same?

Always graph your data to validate assumptions and make sure you are not being misled

# **ALWAYS GRAPH YOUR DATA**

Run charts are important to see if changes occur in a shift, or randomly.

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DATA CLEANING

- Model Outputs are only as good as model inputs.
- Outliers exist. Understanding what to do with them is where you can transform raw data into insights.
- Don't blindly discard the bad data. Ensure that data is reviewed and corrected.
- Site-Specific Range Checks
  - Ensure that data entered will be within a valid range
  - Works best for universal features (i.e. 1.0<pH<14.0)
  - Some data historians have the ability to set conditions when extracting data. [Example Later]

Edit Formatting Rule	?	×
Select a Rule Type:		
← Format all cells based on their values		
← Format only cells that contain		
► Format only top or bottom ranked values		
<ul> <li>Format only values that are above or below average</li> </ul>		
► Format only unique or duplicate values		
► Use a formula to determine which cells to format		
Edit the Rule Description:		
Format only cells with:		
Cell Value v greater than v =\$C\$2		Ť
Preview: AaBbCcYyZz	<u>F</u> orma	ət
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# DATA CLEANING

## **Example – Outlier Calculation**

⊿         Su           172         Mean           1.02         Std De           275         Std Err           263         Upper	mmary S w Mean 95% Mean	tatistics 172.28279 63.17966 1.3038518 174.83962
172         Mean           0.02         Std De           275         Std Err           263         Upper	v Mean 95% Mean	172.28279 63.17966 1.3038518 174.83962
275 Std De 275 Std Err 263 Upper	:v Mean 95% Mean	1.3038518 174.83962
263 Upper	95% Mean	174.83962
75 Lower	05% Mean	160 72507
65 N	5576 Wiedin	2,348
28 N Miss 4.9	sing	656
72		
53 25		
9	128 N Mis 94.9 72 53 25	128 N Missing 94.9 72 53 25

Q = 3 (This can be any number, it just multiplies the outlier distance) Quantile<sub>Low</sub> = 0.25 (25% Quantile) = 128 Quantile<sub>High</sub> = 0.75 (75% Quantile) = 210 Outlier Distance = Q\*(Value(Quantile<sub>(1-x)</sub>) – Value(Quantile<sub>(x)</sub>))

Outlier Distance = 3\*(210-128) = 246

Low Outlier  $\leq$  Value(Quantile<sub>(x)</sub>) - Outlier Distance Low Outlier  $\leq$  128 – 246

Low Outlier  $\leq$  -118 (Here, the obvious case would be to set a minimum outlier value of  $\leq$  **0**)

High Outlier  $\geq$  Value(Quantile<sub>(1-x)</sub>) + Outlier Distance High Outlier  $\geq$  210 + 246 High Outlier  $\geq$  **456** (This is a reasonable value for a high-end outlier)

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# DATA CLEANING

## Setting up Filters in Pi Datalink

2	А	В				
1	EPN	401-T1ENZ-VL 4				
2	Average	0.037422151				
3	Std Dev	0.018518085				
4	High Limit	1.00				
5	Average + 3 Std Dev	0.09				
6	Average - 3 Std Dev	-0.02				
7	Low Limit	0.00				
8						
9	High Filter	0.09				
10	Low Filter	0.00				
11	Filter Expression	'401-" .ENZ-VL'				

Show steps of how to get to the Filter Expression

- 1. For each tag (EPN), set up the average, Std Dev. Pi Calc, cell B2, B3
- 2. Manually set high and low limits in cells B4 and B7.
- 3. Calculate average + 3 Std Dev. Excel formula in Cell B5, B6.
- 4. Set high and low filter as excel equations.
- 1. HIGH = Min(B4, B5)
- 2. LOW = Max(B6:B7)

<"&B9&" AND '"&B1&"' >"&B10

Check with your data historian to see if the filter expression feature is available.

="""&B1&""

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# FEATURE ENGINEERING

Machine learning technique used to create new variables. Used to enhance model accuracy.

- Summary Statistics
  - Mean, Standard Deviation, Min/Max, Median, N
  - Graphing these can show clearer trends than raw data.
- Feature Creation
  - Total Sugars, Ethanol/Solids, Ethanol/Glycerol
  - Supplements raw data going into a model.
  - Improves model accuracy and improves insights for data analytics.

#### Machine Learning Model Buildout



## FEATURE ENGINEERING

Imputation	How to handle missing values. Numeric: Fill in with mean, median, mode. Fix with a calculated value (binned values). Categorical: Label text with "Missing" or "Blank"
Outliers	Remove the values. Quickest method, but the model will lose possibly valuable data. Smart Replace. Impute. Linear regression models susceptible to outliers. Cap value with an arbitrary max or min value based on distribution.
Transform	Log Scale – Convert skewed distributions into a more "normal" distribution. Helps with outliers. Binning – Create intervals that bin the float values into integers. Bins can have varying sizes. Scaling – This normalizes (0-1) or standardizes (0 mean, 1 variance) the range of all features.
One-Hot Encoding Response-Coding	Convert finite data (like categorical) into integers. Works well for Ferm #s, Mash Trains, Trial Conditions. Binary: Converts to 0 or 1. Works well for Pass/Fail, Above/Below average. Use for rare occurrences. Response Coding – creating conditional summary statistics.

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# RANDOMNESS

- Always add randomness to the models, even when evaluating linear regressions.
- Do not assign correlation to features with lower R<sup>2</sup> than random.

Random Normal					(*		
	⊿ Quant	iles		✓ Summary Statistics			
	100.0% 99.5% 97.5% 90.0% 75.0% 50.0% 25.0% 10.0% 2.5% 0.5%	maximum quartile median quartile	3.9723024 2.5697008 1.9473761 1.2726215 0.6783057 0.0124269 -0.667821 -1.275999 -1.951007 -2.52479	Mean Std Dev Std Err Mean Upper 95% Mean Lower 95% Mean N N Missing	0.0041718 0.9953178 0.0053641 0.0146857 -0.006342 34,429 0		
	0.0%	minimum	-3.984277				
Random Uniform					(*		
	⊿ Quant	iles		⊿ 💌 Summary S	tatistics		
	100.0% 99.5% 97.5% 90.0% 75.0% 50.0% 25.0% 10.0% 2.5%	maximum quartile median quartile	0.9999834 0.9947546 0.9749291 0.9012684 0.7518406 0.5043985 0.2558546 0.1023137 0.0260997	Mean Std Dev Std Err Mean Upper 95% Mean Lower 95% Mean N N	0.5026797 0.2879275 0.0015517 0.5057212 0.4996382 34,429 0		
0 02 04 06 00 1	2.070						

# FIT CURVE ANALYSIS

## Trend any HPLC analyte across fermentation time.

Better understand fermentation kinetics.



Great way to incorporate feature engineering into models. For Ethanol, get information like:

**Inflection point** – when ethanol production rate of growth is negative.

Asymptote – Peak ethanol values based on the curve.

# PROCESS SCREENING

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# PROCESS SCREENING

- Process Screening Setup can be scripted for Fermentation.
- Good practice to have a data filter for Month/Year to see local changes.



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## **PROCESS SCREENING**



#### Sort Features by Stability

	v
Column	Stability Index
%Lactic	3.33
Delta Acetic	2.45
%DP3	2.10
%DP1	2.08
Temp	1.94
%Total Sugars	1.88
%DP2	1.84
%Glycerol	1.65
pН	1.56
Brix	1.45
%DP4+	1.39
Delta Glycerol	1.35
%Acetic	1.32
Delta Lactic	1.27



## **PROCESS SCREENING**

### **Nelson Rules**



# PREDICTOR SCREENING

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Batch #

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# SCREENING FOR IMPORTANT VARIABLES

#### **Predictor Screening**



- Quickly go from many variables to find the most important variables, or the ones that correlate with the target.
- Include Random Uniform and Random Normal in the screening. Focus on variables above Random.

# VARIABILITY ANALYSIS

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Case Study

# VARIABILITY ANALYSIS

### **Overview**

#### Goal

Estimate how much of the variability in the selected performance metric is stemming from each product type, and how big the residual is for a specific dataset.

#### Model

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A **linear mixed model** is generalization of a linear regression model, where the mixed model can also take grouping in the data into account.

#### Assumption

Random effect coefficients and residuals are drawn from a normal distribution. The variance of this normal distributions tells us how much of the variability in data can be assigned to that grouping.



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Image source: https://towardsdatascience.com/how-linear-mixed-model-works-350950a82911

# EXAMPLE: LINEAR MIXED MODEL

## Grouping: Yeast type

Here Ethanol Drop is the y-metric, Ferm solids is the fixed effect, and Yeast Type is the Random effect, adding a type dependent **random intercept**.

These random intercepts are drawn from a normal distribution. The variance of the normal distribution compared to the unexplained variability left in Ethanol Drop, tells us how much of the variability in Ethanol drop, not accounted for by Ferm Solids, can be accounted for by the Yeast type.

This chart shows which yeast types performed better. Let's discover what else are the core drivers of performance.



# EXAMPLE: LINEAR MIXED MODEL

## **Grouping: Yeast**

After a fit to Ferm Solids, variability left in Ethanol Drop is attributed to

- 47% Prop Add Yest Type
- 53% Residual

Residual will include other product changes, as well as process changes, corn quality changes etc.

It should be considered that process changes aligned in time with Yeast Type changes, will appear as an effect of the Yeast Type. This is why multiple changes during product trials make results tricky to interpret!

Variance Component Estimates are based on a model fit to historical data. Hence changes in data or in the model construction will change the outcome.

If we want to further understand how **other products** or interactions between products impact the performance, we need to include all products in the linear mixed model (see next slide).

Core driver of process variability	Description	Size of Variability
Yeast	Variability in Ethanol caused by differences between Yeasts	47%
Residual: Process parameters, Corn quality, etc.	Differences in Ethanol caused by all other features.	53%

## LINEAR MIXED MODEL: INCL. ALL PRODUCTS

#### A REML Variance Component Estimates

Dan dam Effect	
CA Turne	2 059
GA Type	1 277
Prem Add Anubioucs Type	10.022
Prop Add Yeast Type	19.932
Prop Add Anubioucs Type	0.000
Prop Adds Prop GA Type CA Type*Form Add Antibiotics Type*Deen Adds Deen CA Type*Deen Add Antibiotics Type*Deen Add Veest Type	0.000
GA Type"Perm Add Antibiotics Type"Prop Adds Prop GA Type"Prop Add Antibiotics Type"Prop Add Yeast Type	2.980
GA Type"Ferm Add Antibiotics Type	0.000
GA Type^Prop Adds Prop GA Type	0.220
Ferm Add Antibiotics Type*Prop Adds Prop GA Type	0.030
GA Type*Ferm Add Antibiotics Type*Prop Adds Prop GA Type	0.451
GA Type*Prop Add Antibiotics Type	0.000
Ferm Add Antibiotics Type*Prop Add Antibiotics Type	0.000
GA Type*Ferm Add Antibiotics Type*Prop Add Antibiotics Type	4.967
Prop Adds Prop GA Type*Prop Add Antibiotics Type	2.205
GA Type*Prop Adds Prop GA Type*Prop Add Antibiotics Type	1.793
Ferm Add Antibiotics Type*Prop Adds Prop GA Type*Prop Add Antibiotics Type	0.000
GA Type*Ferm Add Antibiotics Type*Prop Adds Prop GA Type*Prop Add Antibiotics Type	0.000
GA Type*Prop Add Yeast Type	0.000
Ferm Add Antibiotics Type*Prop Add Yeast Type	0.000
GA Type*Ferm Add Antibiotics Type*Prop Add Yeast Type	2.352
Prop Adds Prop GA Type*Prop Add Yeast Type	17.266
GA Type*Prop Adds Prop GA Type*Prop Add Yeast Type	0.000
Ferm Add Antibiotics Type*Prop Adds Prop GA Type*Prop Add Yeast Type	0.000
GA Type*Ferm Add Antibiotics Type*Prop Adds Prop GA Type*Prop Add Yeast Type	0.000
Prop Add Antibiotics Type*Prop Add Yeast Type	9.818
GA Type*Prop Add Antibiotics Type*Prop Add Yeast Type	0.000
Ferm Add Antibiotics Type*Prop Add Antibiotics Type*Prop Add Yeast Type	0.014
GA Type*Ferm Add Antibiotics Type*Prop Add Antibiotics Type*Prop Add Yeast Type	0.000
Prop Adds Prop GA Type*Prop Add Antibiotics Type*Prop Add Yeast Type	0.000
GA Type*Prop Adds Prop GA Type*Prop Add Antibiotics Type*Prop Add Yeast Type	2.113
Ferm Add Antibiotics Type*Prop Adds Prop GA Type*Prop Add Antibiotics Type*Prop Add Yeast Type	6.549
Residual	24.970
Total	100.000

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# LINEAR MIXED MODEL: ALL PRODUCTS

## Core drivers of ETHANOL variability

Core driver of process variability	ţĊ	Description	Size of Variability	Model insights
Yeast		Variability in Ethanol caused by differences between Yeasts		• Yeast is a key driver of process variability.
GA*Yeast		Variability in Ethanol caused by differences in the specific combination of GA and Yeast	47%	<ul> <li>The interaction between yeast and GA type is a key driver of process variability.</li> </ul>
Antibiotics*Yeast		Variability in Ethanol caused by differences in the specific combination of Antibiotics and Yeast		<ul> <li>The interaction between yeast and Antibiotics also has some impact on process variability, though significantly less than yeast and GA type combination.</li> </ul>
Residual: Process parameters, Corn quality, etc.		Differences in Ethanol caused by the process conditions and corn quality differences.	25%	<ul> <li>Process setpoints are not consistently achieved in production and tend to have variation in fermentation time, percent backset and more.</li> <li>Corn quality is not well accounted for. It could potentially be a big unknown driver of ethanol variability</li> </ul>

# CREATE YOUR OWN LEAST SQUARES LINEAR MODELS

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# LEAST SQUARES LINEAR MODEL

### Find the most impactful features

One feature	Two features	Multiple features
Y = mx+b	$Y = m_1 x_1 + m_2 x_2 + b$	$Y = b + m_1 x_1 + m_2 x_2 + \dots$

Each feature individually has a poor linear fit with ethanol yield. How can you make a formula that fits all of these features into one equation?



# LEAST SQUARE MODELS

## Setup in Microsoft® Excel®

True = Calculated y-intercept FALSE = y-intercept = 0

Each feature should be one column.

The Y-metric should also be a column.

Formula = LINEST([known\_ys],[known\_xs],TRUE,TRUE)

[Known\_ys] will be the column of the Y metric [known\_xs] can be 1 or multiple columns of features

The output table will be 4 rows by and span all columns.

True = Full statistics table FALSE = slope and y-intercept only

> Let's do an example. How well can we predict Ethanol/Solids based on 12-hr HPLC + Solids?

# LEAST SQUARE MODELS

## Early Ferm Example Setup

× ✓ f<sub>x</sub> =LINEST(C8:C215,D8:N215,TRUE,TRUE) Formula



# LEAST SQUARE MODELS

## Early Ferm Example Setup

X ✓ f<sub>x</sub> =LINEST(C8:C215,D8:N215,TRUE,TRUE)

#### Slopes are in reverse order of features!

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	Α	В	С	D	E	F	G	Н		J	К	L	М	Ν	<b>/-Interce</b>
1			Slopes	-0.16295	-0.02186	0.051117	0.03916	-0.01938	0.023773	0.012179	0.009681609	2.20016E-06	0.001208	-0.01501	0.237098
2		Stand	dard Error	0.030747	0.017902	0.005472	0.00239	0.005329	0.003866	0.002823	0.00146896	0.000161237	0.001519	0.001678	0.056984
3			R <sup>2</sup> Value	0.725107	0.033067	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A
4			F Value	47.00031	196	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A
5			RSS	0.565302	0.21431	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A
6															
7	Batch	Hour	Yield	Liq Solids	Backset So	Age	Fill Time	DP1	DP2	DP3	DP4	Ethanol	Glycerol	Lactic	
8	1257	12Hr	0.40	<u>.</u> 32,30	920	53.75	-10.17	51.657	1.5.6.24	A. 44.42	1		4- 9.54	1. 1. 1. 1. 2.	
9	1258	12Hr	0.39		1. 9. RO	8 59-60	8 4 19 58	K -25.6	国际历历	× 416	Part of the set		×, 6, 49	1. S. W.O.	
10	1259	12Hr	0.42	32,90	0 45.10	13 24 95	1000	1915 38	0.16	ST 1938	1. S. O. M. 17	5.5 8 2.01	A.S. 16 43	0.16	
11	1263	12Hr	0.43	30.38	7. 440	1. 55.42	2 40.73	語な	eatu	ires		1. 2 2.86	金油	0.13	
12	1264	12Hr	0.43	196.45	9.10	19 6 4	10.07	146.82	4月1日開設7	× 1. 43:48	64. 82		1153	6 2 0.23	
		1	Y-Metric												i

#### **RSS** = Regression of sum of squares

# LEAST SQUARE MODELS

## Early Ferm Example Setup

X ✓ f<sub>x</sub> =LINEST(C8:C215,D8:N215,TRUE,TRUE)



# LEAST SQUARE MODELS

### Results



What can you do with results:

- Plot how changing certain features affect average performance.
- Interpret which features have the largest impact on performance (largest slope).
- Rerun model over time and see how the results shift.
- Create models specific to certain products to optimize various features.

# PERFORMANCE METRIC EVALUATION

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## **PERFORMANCE METRIC SELECTION**



Minimize the deviation in your metric for better insights.

Evaluate multiple metrics; basic and advanced.

Evaluating the best metric allows for the most success with product trials and process changes.

**Features** 



Metric ordered by RSquare (ascending)

# TRIAL EVALUATION

## Z-test in Microsoft® Excel®

#### Inputs & Results:

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			A	B	C	D	E	F	(	3	Н
		1		baseline	trial						
		2		13	13.1						
		3		13.1	13.2						
nts 🖻 S	hare	4		13.5	13.6						
ata Analysis		5		12.8	12.9	z-Test: T	wo Sample f	or Means			
lver	-	6		12.9	13	Input					
		7	Variance	0.0584	0.0584	Variabl	e <u>1</u> Range:		SB\$1:SB	56	<u>↑</u>
		8				Variabl	e <u>2</u> Range:		SCS1:SC	\$6	Î
Analyze		9	z-Test: Two Sample for Means					Diff			
		10				Hypoth	esized Mean	Differenc	e: 0.1	1	
		11		baseline	trial	Variabl	e 1 <u>V</u> ariance	(known):	0.0	)584	
Р	C	12	Mean	13.06	13.16	Variabl	e 2 Variance	(known):	0.0	)584	
		13	Known Variance	0.0584	0.0584		<u>-</u>		0.0	504	
		14	Observations	5	5	<u> </u>	els				
		15	Hypothesized Mean Difference	0.1		<u>A</u> lpha:	0.05				
		16	Z	-1.31		Output	ontions				
		17	P(Z<=z) one-tail	0.10			put Papaci		\$459		1
		18	z Critical one-tail	1.64			put Kange:	Dha			<u> </u>
		19	P(Z<=z) two-tail	0.19		ONev	v worksneet	<u>P</u> I <b>y</b> :			
		20	z Critical two-tail	1.96		O Nev	V <u>W</u> orkbook				
						-					

Based on the two-tail p-value, we can conclude with 81% certainty that the trial data exceeds the baseline data by 0.1.

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#### To access:

					μC	comments 🛛 🖻 Sh	are
nsolidate Data Model ~	What-If Forecast Analysis ~ Sheet	Group	Ungroup V	Subtotal	+     	☐ Data Analysis ?→ Solver	
	Forecast		Outline		ы	Analyze	
Data Analysis <u>A</u> nalysis Tools Histogram Moving Average Random Number Generation Rank and Percentile Regression Sampling t-Test: Paired Two Sample for Means t-Test: Two-Sample Assuming Equal Variances t-Test: Two-Sample Assuming Unequal Variances <u>z-Test: Two Sample for Means</u>			?	X OK Cancel <u>H</u> elp	C	) P	C

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# PROCESS UNIT MACHINE LEARNING

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# **PROCESS UNIT MACHINE LEARNING**

### Interactions



In this model: Liq Solids and Slurry Temperature have the highest interaction value.

Interaction is 50% higher than the second highest interaction.

# **PROCESS UNIT MACHINE LEARNING**



# Feature Effect Interaction Effect

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# **PROCESS UNIT MACHINE LEARNING**



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## How it Works

Create a report of all available prop data, gathering data at 15-minute intervals. Each prop is given a unique ID consisting of tub name, date, and hour of set time.

Create 5 distinct phases, based on the tub level, temperature, temperature controller output, and rate of change (direction and magnitude).

Phases:

1 = WashFind a better way to evaluate time-series data by<br/>overlaying all prop batches.2 = EmptyThen separate the prop duration into phases to<br/>evaluate separately.3 = Fillevaluate separately.

- 5 = Drop

## **HOW IT WORKS**



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Date



Evaluating props based on time can be difficult. The cumulative times do not always line up.

To best evaluate these phases, we need to group these phases based on relative time (phase time).



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By evaluating each phase of each prop by completeness, we have a better understanding of which features have the largest impact. This process of phasing the prop time is called "dynamic time warping".

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Now, instead of feeding *prop hours* into the model, we can use the better *phase hours*.

Phase hours also lets us evaluate each phase individually.

## **Model Results**

Gain insights on more than just HPLC from a couple of samples per prop.

Analyze adjustments to both products and process at the same time.

If the goal is viable cell count, what levers can we pull to collectively raise the cell count enough to decrease yeast volume pitched?





## **SUMMARY**

#### What Can YOU Do?

Data Upload/Cleaning Feature Engineering Least Square Linear Models Trial Evaluation

#### What Can I Do?

Automated Data Reporting Process Screening Fit Curve Analysis Power Explorer/Trial Evaluation

#### What Can Al Do?

Predictor Screening Variability Analysis Partition Models Trained/Validated Models Dynamic Time Warping



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