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X C E L I S ® A I 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

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)

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OBJECTIVES

What is the goal of the talk today?

What can *you* **do for you?**

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What can *I* **do for you? What can** *AI* **do for you?**

OBJECTIVES

Data Cleaning and Outlier Analysis **Batch Linking Model Evaluation** Batch Linking Model Evaluation

Least Square Linear Models Residence Entert Models
(Multiple Features) Multiple Features and Dynamic Time Warping

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Data Upload **Performance Metric Evaluation** Trained/Validated ML Models

Feature Engineering **Direct/Indirect Feature Analysis Local Data Analysis Communist Engineering**

Predictor Screening, Partition **Modeling**

Process Screening **Fit Curve Analysis** Probabilistic Action Items

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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]

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DATA CLEANING

Example – Outlier Calculation

Q = 3 (This can be any number, it just multiplies the outlier distance) QuantileLow = 0.25 (25% Quantile) = 128 QuantileHigh = 0.75 (75% Quantile) = 210 Outlier Distance = Q*(Value(Quantile(1-x)) – Value(Quantile(x)))

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

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Low Outlier ≤ Value(Quantile_(x)) - Outlier Distance Low Outlier ≤ 128 – 246

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

High Outlier \geq Value(Quantile_(1-x)) + Outlier Distance High Outlier $\geq 210 + 246$ High Outlier ≥ **456** (This is a reasonable value for a high-end outlier)

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DATA CLEANING

Setting up Filters in Pi Datalink

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&"'

FEATURE ENGINEERING

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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

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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^2 than random.

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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

PROCESS SCREENING Nelson Rules

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PREDICTOR SCREENING

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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.

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VARIABILITY ANALYSIS

Case Study

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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

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.

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).

LINEAR MIXED MODEL: INCL. ALL PRODUCTS

△ REML Variance Component Estimates

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LINEAR MIXED MODEL: ALL PRODUCTS

Core drivers of ETHANOL variability

CREATE YOUR OWN LEAST SQUARES LINEAR MODELS

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LEAST SQUARES LINEAR MODEL

Find the most impactful features

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?**

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LEAST SQUARE MODELS

Early Ferm Example Setup

Formula =LINEST(C8:C215,D8:N215,TRUE,TRUE) \times \checkmark fx

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LEAST SQUARE MODELS

Early Ferm Example Setup

 \times \checkmark fx =LINEST(C8:C215,D8:N215,TRUE,TRUE)

Slopes are in reverse order of features!

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RSS = Regression of sum of squares

LEAST SQUARE MODELS

Early Ferm Example Setup

=LINEST(C8:C215,D8:N215,TRUE,TRUE) \checkmark fx \times

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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

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Outline

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Z-test in Microsoft® Excel®

To access:

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Data

Model ~

Data Analysis

Analysis Tools

Moving Average

Rank and Percentile

Random Number Generation

Z-Test: Two Sample for Means

t-Test: Paired Two Sample for Means t-Test: Two-Sample Assuming Equal Variances t-Test: Two-Sample Assuming Unequal Variances

Histogram

Regression Sampling

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What-If Forecast

Analysis v Sheet

Forecast

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Inputs & Results:

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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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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DYNAMIC TIME WARPING

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DYNAMIC TIME WARPING

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 = Wash

2 = Empty

 $3 =$ Fill

4 = Prop

5 = Drop

Find a better way to evaluate time-series data by overlaying all prop batches.

Then separate the prop duration into phases to evaluate separately.

HOW IT WORKS

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DYNAMIC TIME WARPING

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).

DYNAMIC TIME WARPING

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.

DYNAMIC TIME WARPING

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 AI Do?

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

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