Predicting complex industrial processes using Sparse Regression Models

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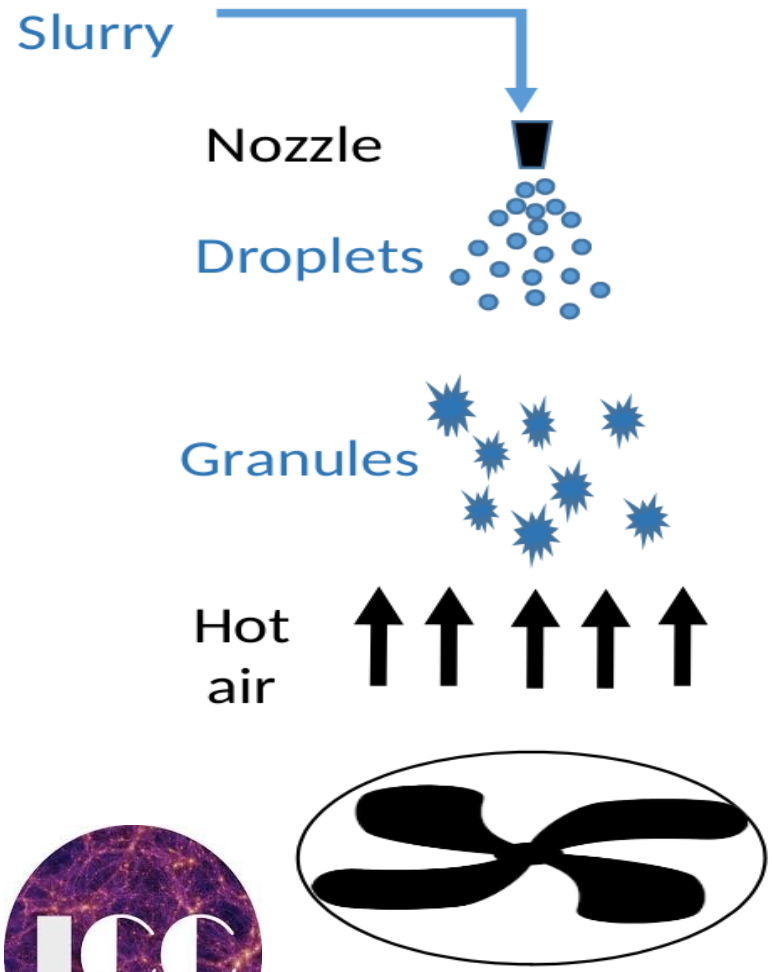
The problem: Predicting physical characteristics of a spray drying process for laundry powder.



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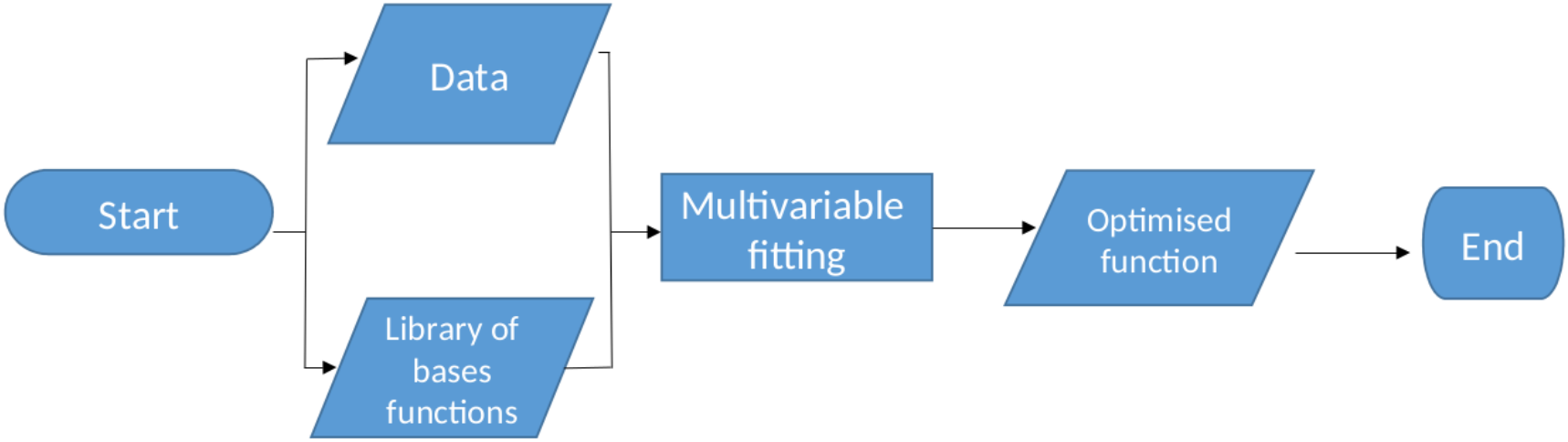
Our task: Finding the optimal parameters.

$$Property(x_{1,\ldots},x_n) = a_0 \cdot f_0(x_{1,\ldots},x_n) + \ldots + a_m \cdot f_m(x_{1,\ldots},x_n)$$

Ingredients and Process Conditions

Parameters from the linear combination of bases functions



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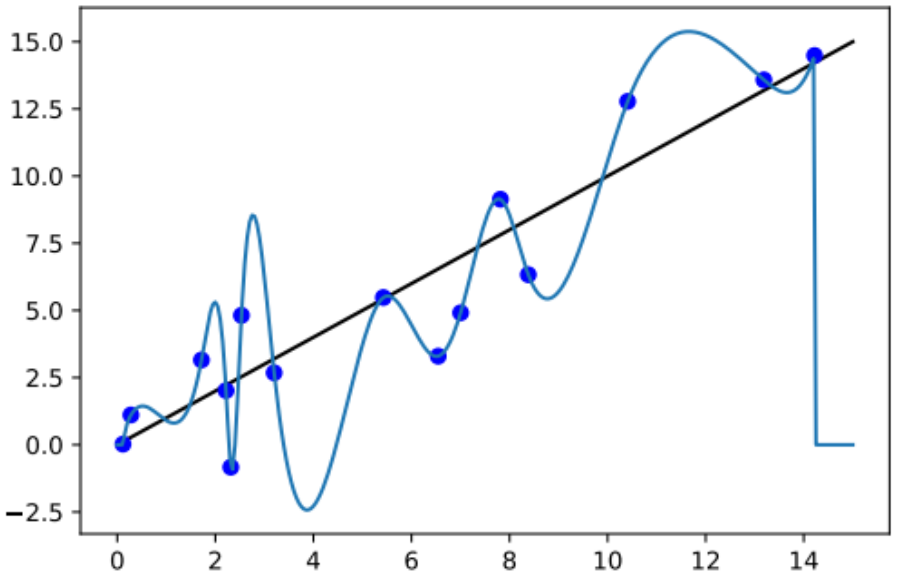
Model: 13-20 Independent variables combined in hundreds of functional forms.

100-1000 Parameters!!!!!

Data: ~300 points!!!

We have to be very careful with overfitting.



The blue points are fitted by two different models the turquoise line is a perfect fit to the data but it is difficult to justify. The black line while being the worst fit is simple and more realistic.

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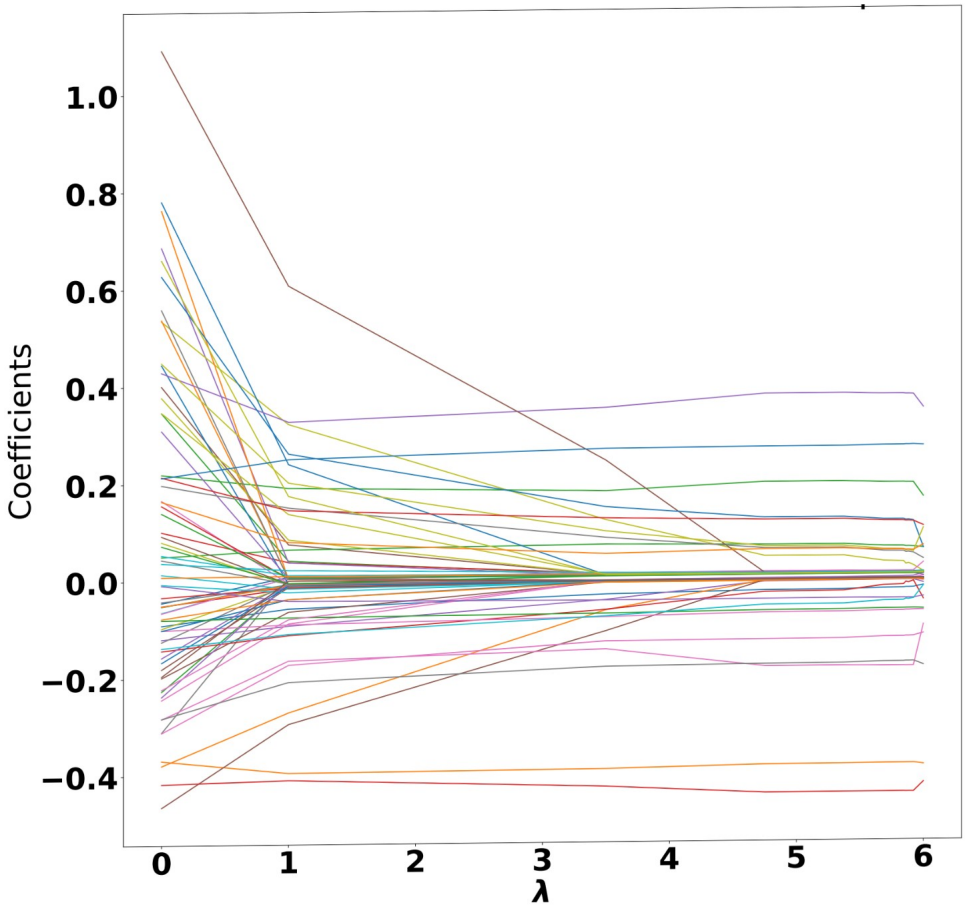
Solution: Sparse regression with a penalty function.

$$L = \frac{1}{N}\sum_{i=0}^{M}\left(y_i - f\left(x_i\right)\right)^2 + \lambda \times Penalty_{NDA}$$



Best fit normalized coefficients as a function of the penalty parameter.

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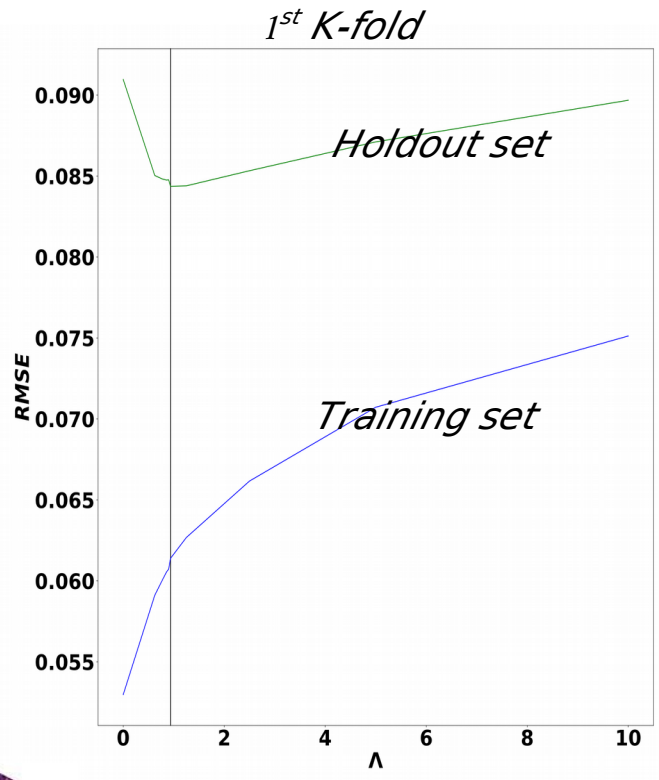
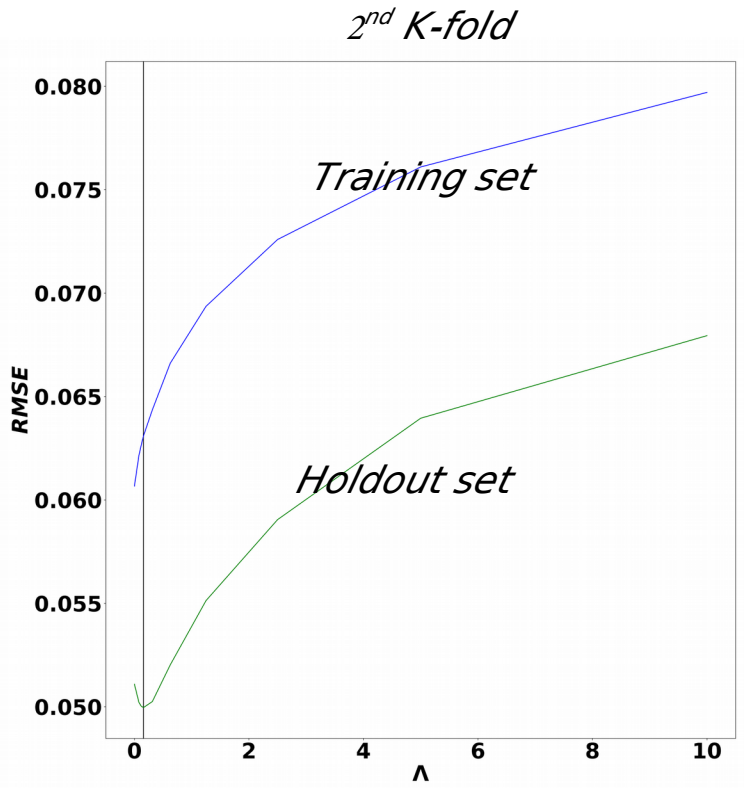
Standard Penalty selection method (k-folds) is too unstable.





The K-folds method divides the data into N fractions. One of them is selected as a Holdout set and is systematically kept out of the fit.

Solution: Use mock data sets (Icaza-Lizaola et al. In prep).

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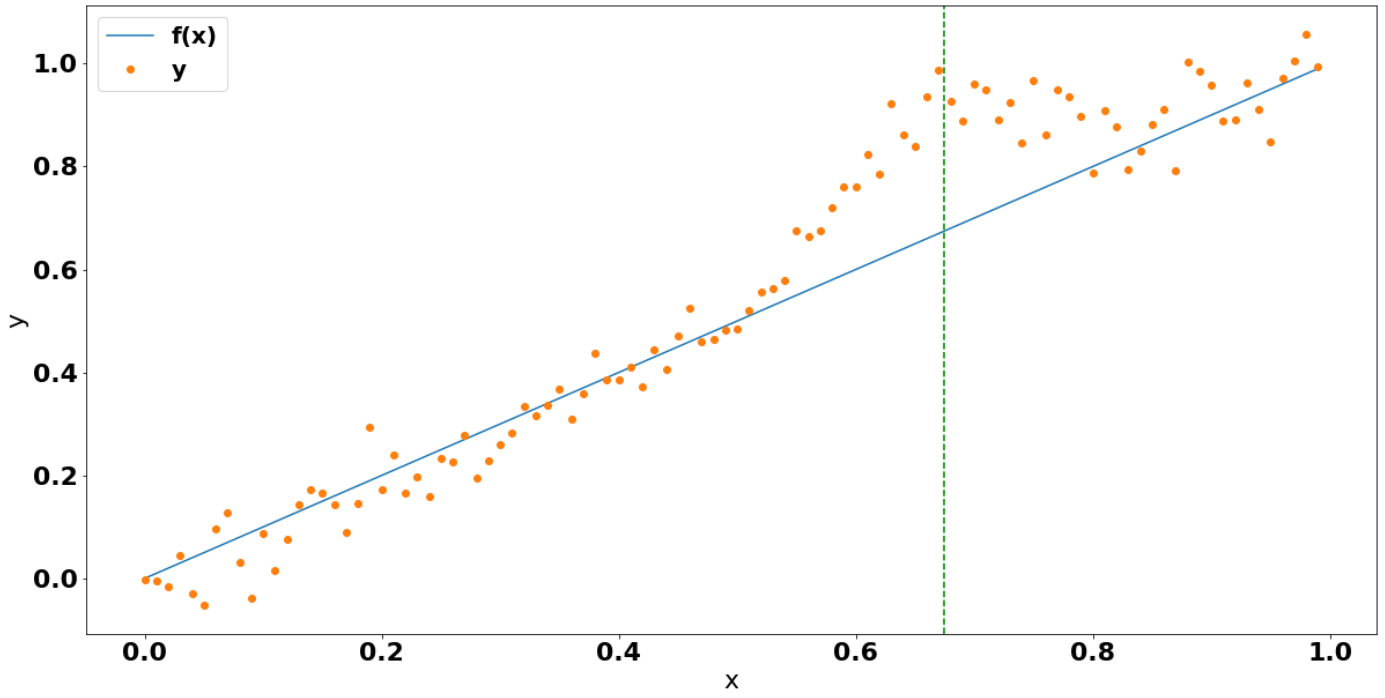
Sparce regression models the global behavior properly, but **Gaussian Emulators** can be used to improve local deviations.



Example of one data set fitted by a model (Blue line) where the global behavior is properly explained, but local deviations would not be modeled.

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Conclusions

-We developed an automatized methodology that is able to model P&Gs spray drying tower parameters.

-Our sparse regression model has similar accuracy to that obtained by P&G chemical engineers.

-When enough data is included Gaussian Emulators make our code more accurate than previous P&G models. However, the lack of a functional form makes it harder to interpret.

-We are currently using our methodology to try to predict the Mass of a galaxy inside a Dark Mater halo.

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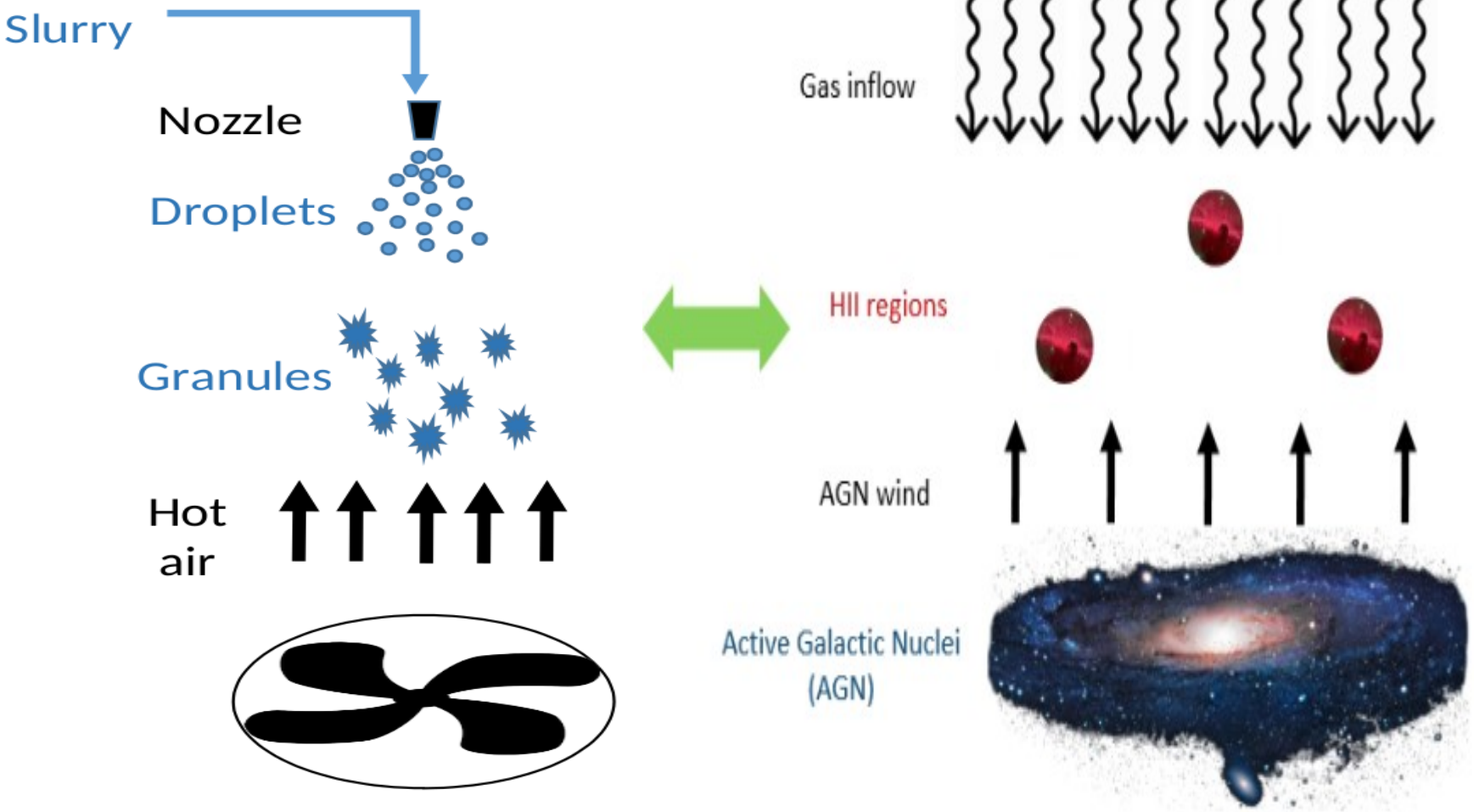

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