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We will begin our presentation in a few minutes…

STEVENS
INSTITUTE of TECHNOLOGY
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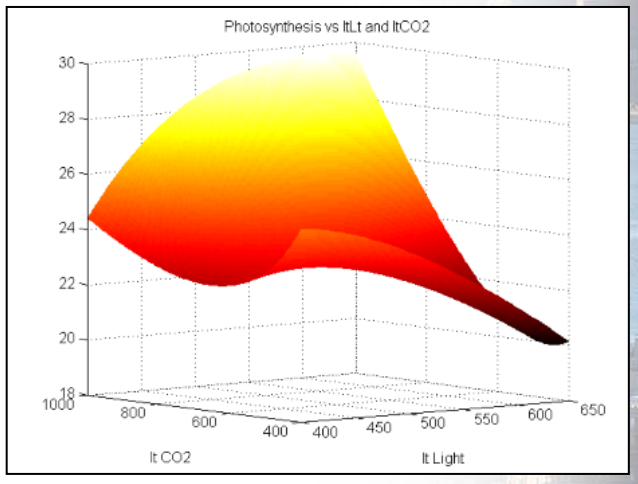
Modeling Complex Environmental Data Without the Black Box

Multivariate Polynomial Regression

AAEES Webinar
February 16, 2022



David A. Vaccari
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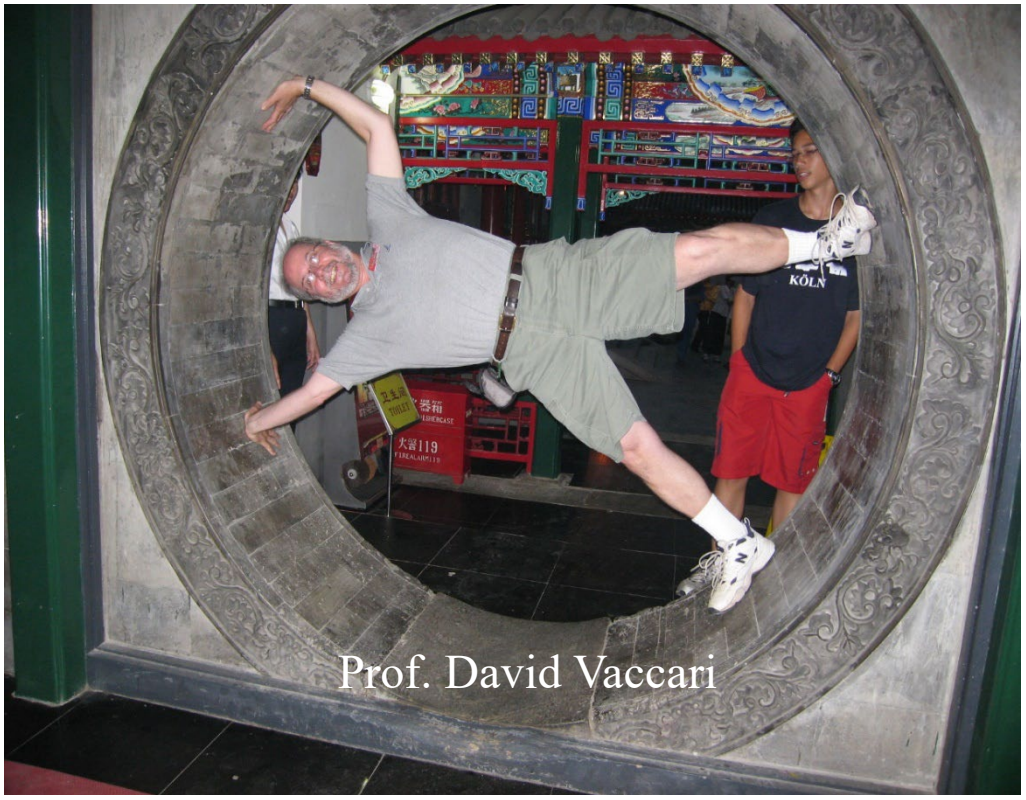


Prof. David Vaccari

Environmental Engineer specializing in:

- Wastewater treatment
- Statistical modeling
- Phosphorus resources

Rutgers University:

- Environmental science
- Chemical engineering

Stevens Institute of Technology:

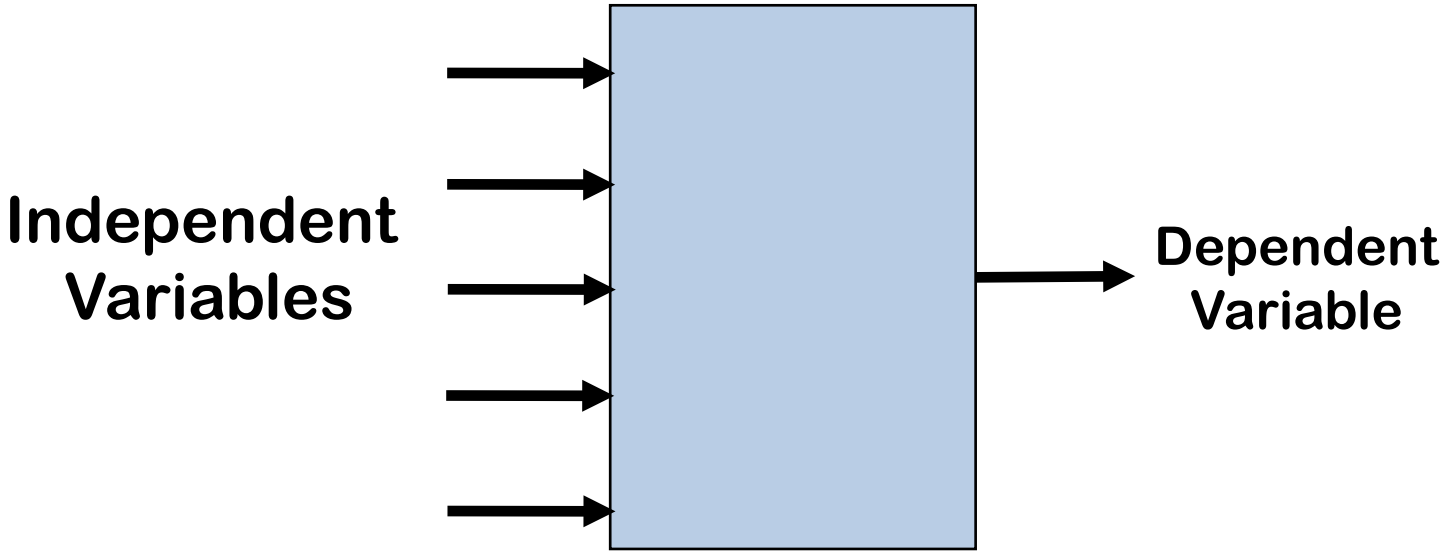
- Professor of environmental engineering

- Licensed Professional Engineer
- Board-Certified Environmental Engineer
- President-elect, AAEES
- Fellow of ASCE

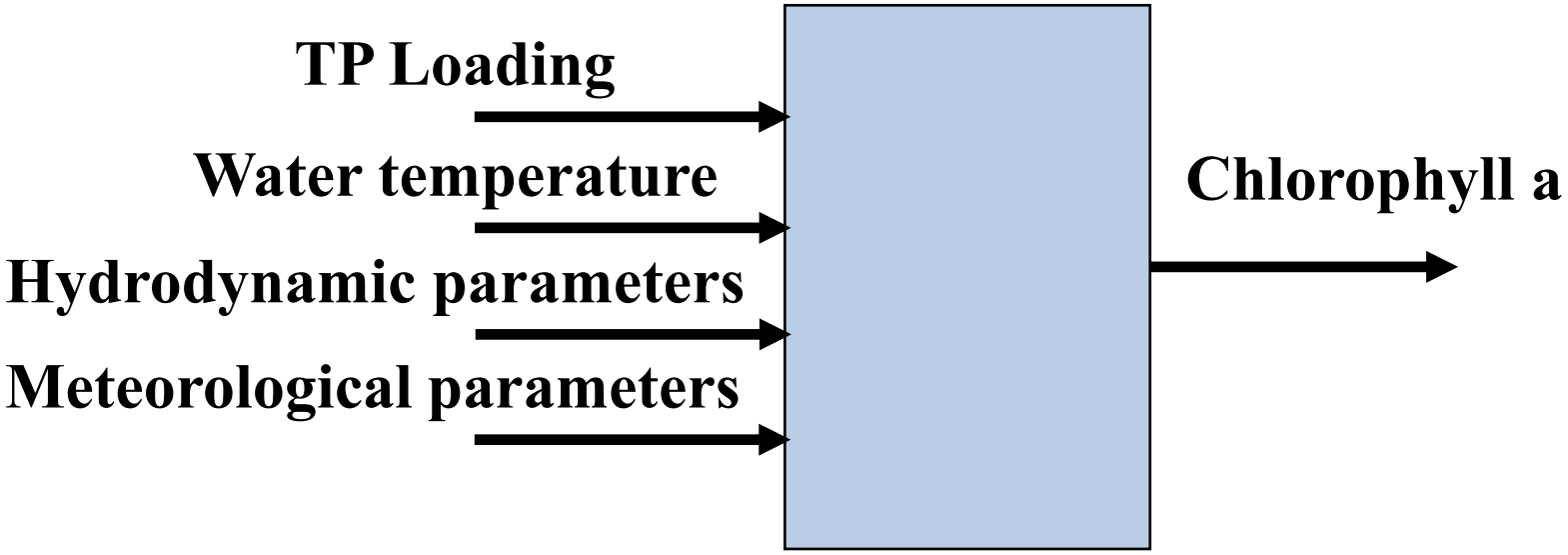
Outline

1. Introduction – modeling approaches
    - Artificial Neural Networks
    - Simple Linear Regression (review) and Goodness-of-Fit
    - Multilinear Regression
2. Multivariate Polynomial Regression
3. *TaylorFit* – Overview and features
    - Cross-validation and Final validation
    - Model analysis – residuals and sensitivity analysis
    - Confidence intervals and Prediction Intervals
4. Example applications
    - Macrophyte Indices
    - Photosynthetic productivity for NASA
    - Phytoplankton occurrence in the Hudson and East Rivers
    - Retail Industrial Sales

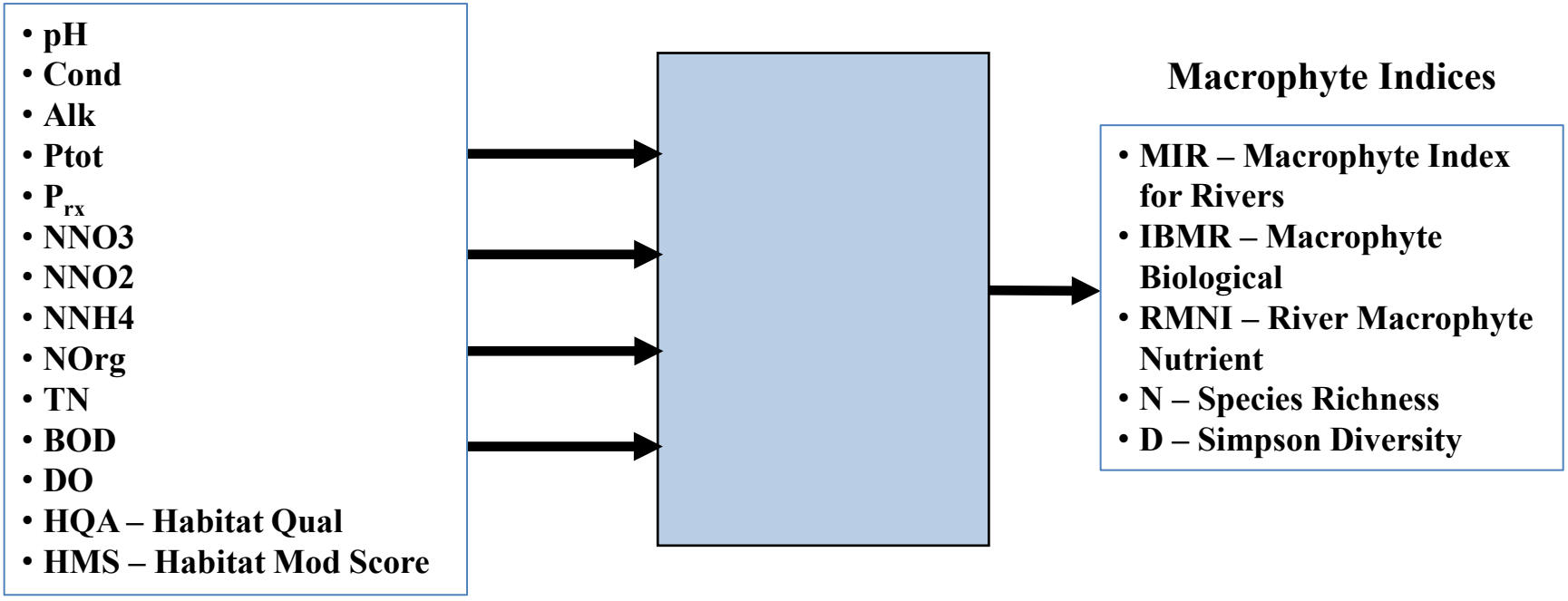
The Problem of Multivariable Correlation and Complexity



Water Quality

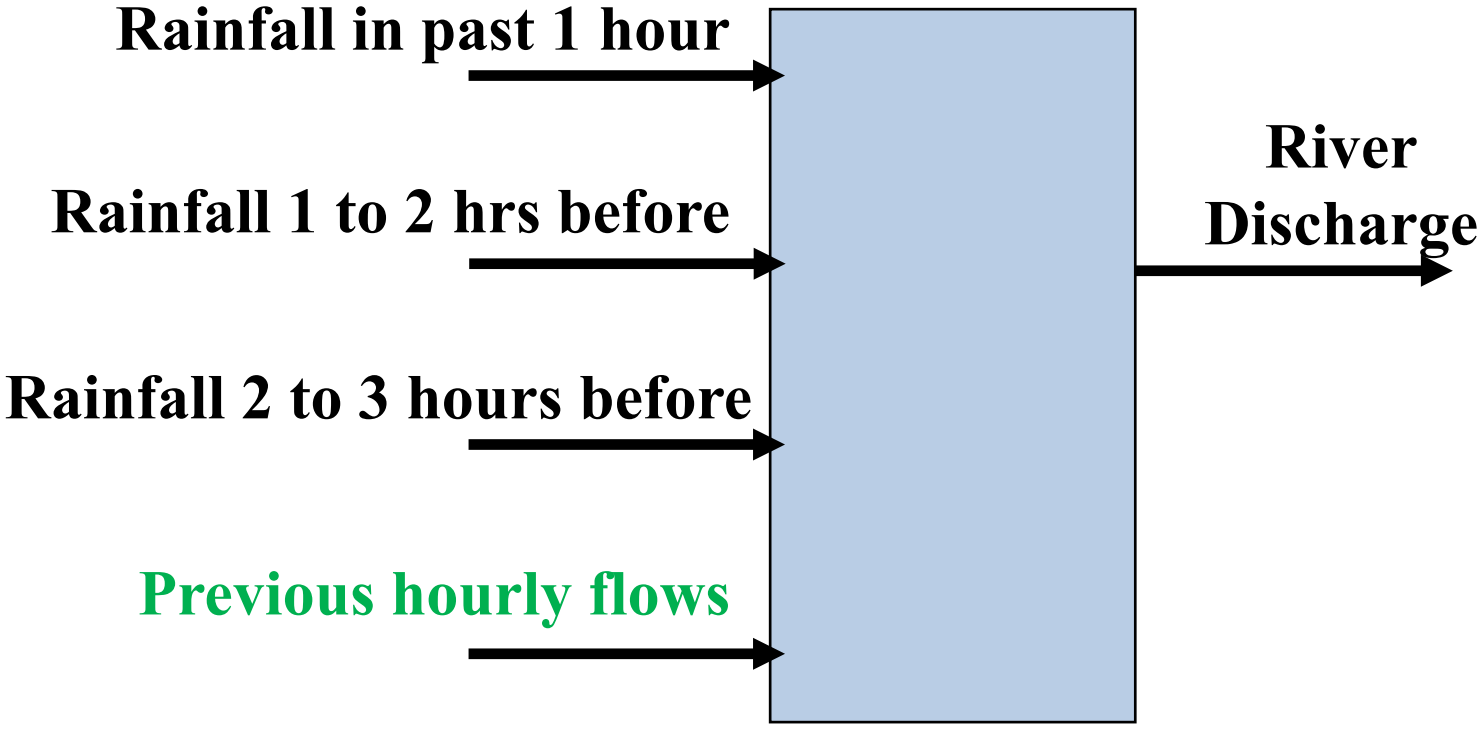


Water Quality



Vishwa Shah, Sarath Chandra K. Jagupilla *, David A. Vaccari, Daniel Gebler (2021). Non-Linear Visualization and Importance Ratio Analysis of Multivariate Polynomial Regression Ecological Models based on River Hydromorphology and Water Quality. Section: Ecohydrology, *Water* 2021, 13, 2708. https://doi.org/10.3390/w13192708.

Time-Series Example



Predictive Modeling Approaches

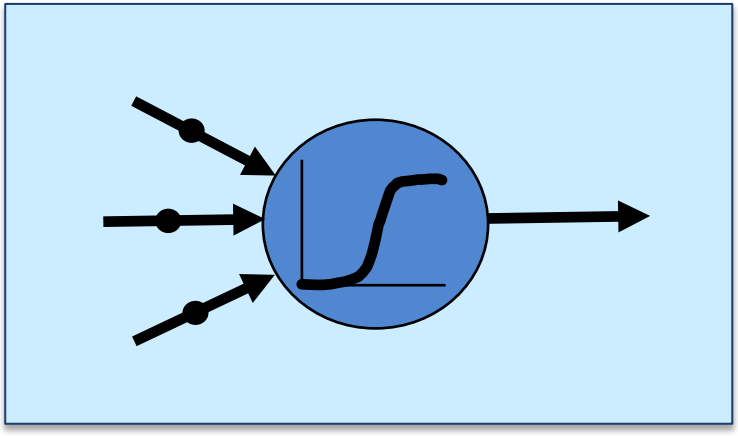
Linear

- Multilinear Regression (MLR)

Nonlinear

- Artificial Neural Networks (ANNs)
- Multivariate Polynomial Regression (MPR)

Artificial Neural Networks



Artificial Neural Networks

Pros

- Accurate
- Describes complex behavior
- Handles high dimensional problems

Cons

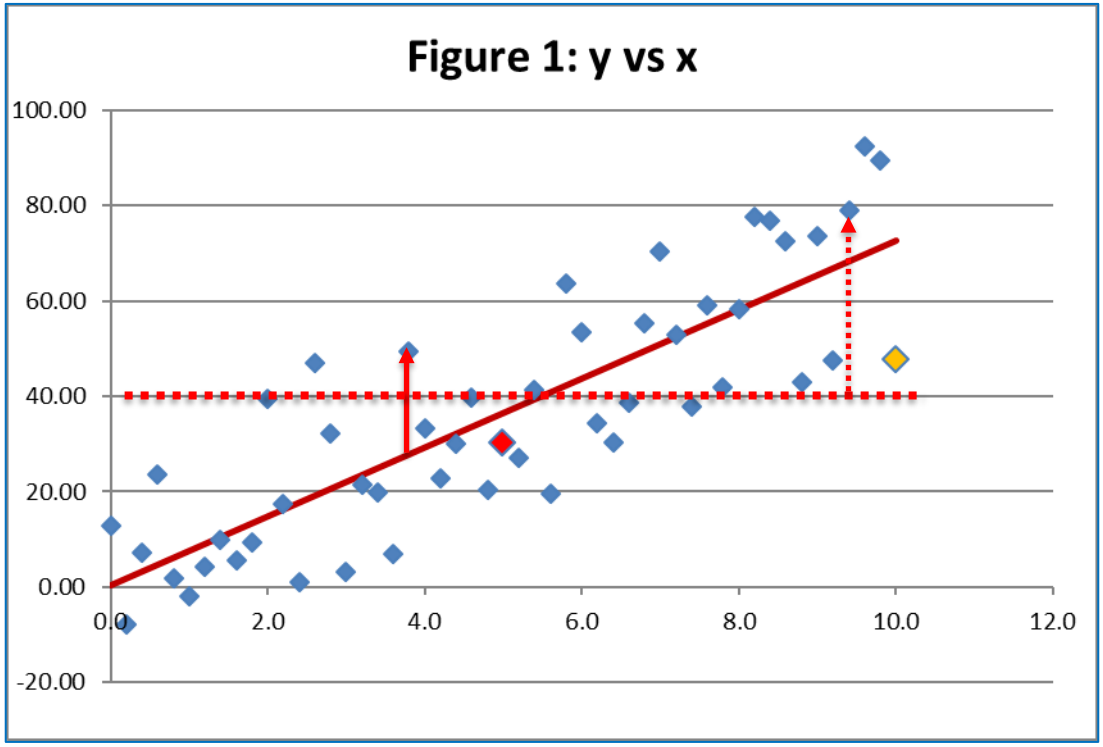
- Complex
- Difficult to analyze
- Difficult to communicate
- Susceptible to overfitting
- Hidden behavior: **Black Box!**

Simple Linear Regression

Optimization problem:
Find slope and intercept that minimize the Sum of Squares of the Error (SSE)

TSS is sum of squares of deviation from the mean

$$0 < SSE < TSS$$



Worst case: SSE = TSS

I.e., if x provides no predictive power

And, of course, the "best" outcome would be SSE = 0

Our first Global Goodness-of-Fit Statistic

$$R^2 = 1 - \frac{SSE}{TSS}$$

$$0.0 \leq R^2 \leq 1.0 \quad \textbf{(}\textbf{\textit{for }}\textbf{\textit{\underline{fit}}}\textbf{ only)}$$

Interpretation:
Approximately the fraction of the variance in y that is explained by the model

Multilinear Regression (MLR)

- MLR model

$$y = a_0 + a_1 \cdot x_1 + a_2 \cdot x_2 + a_3 \cdot x_3 + \ldots a_n \cdot x_n$$

- Problem of always increasing R^2

How do you determine how good is good enough?

- GOF statistics that penalize complexity
- Parsimonious selection of terms based on *t*-statistic

Global GoF Statistics that Penalize Complexity

- All are based on ***TSS, SSE, n_d, n_p***

$$R^2 = 1 - \frac{SSE}{TSS}$$

$$df = n_d - n_p$$

$$SSR = TSS - SSE$$

$$TMS = \frac{TSS}{n_d - 1}$$

$$MSE = \frac{SSE}{df}$$

$$MSR = \frac{SSR}{n_p}$$

$$R^2_{adj} = 1 - \frac{MSE}{TMS}$$

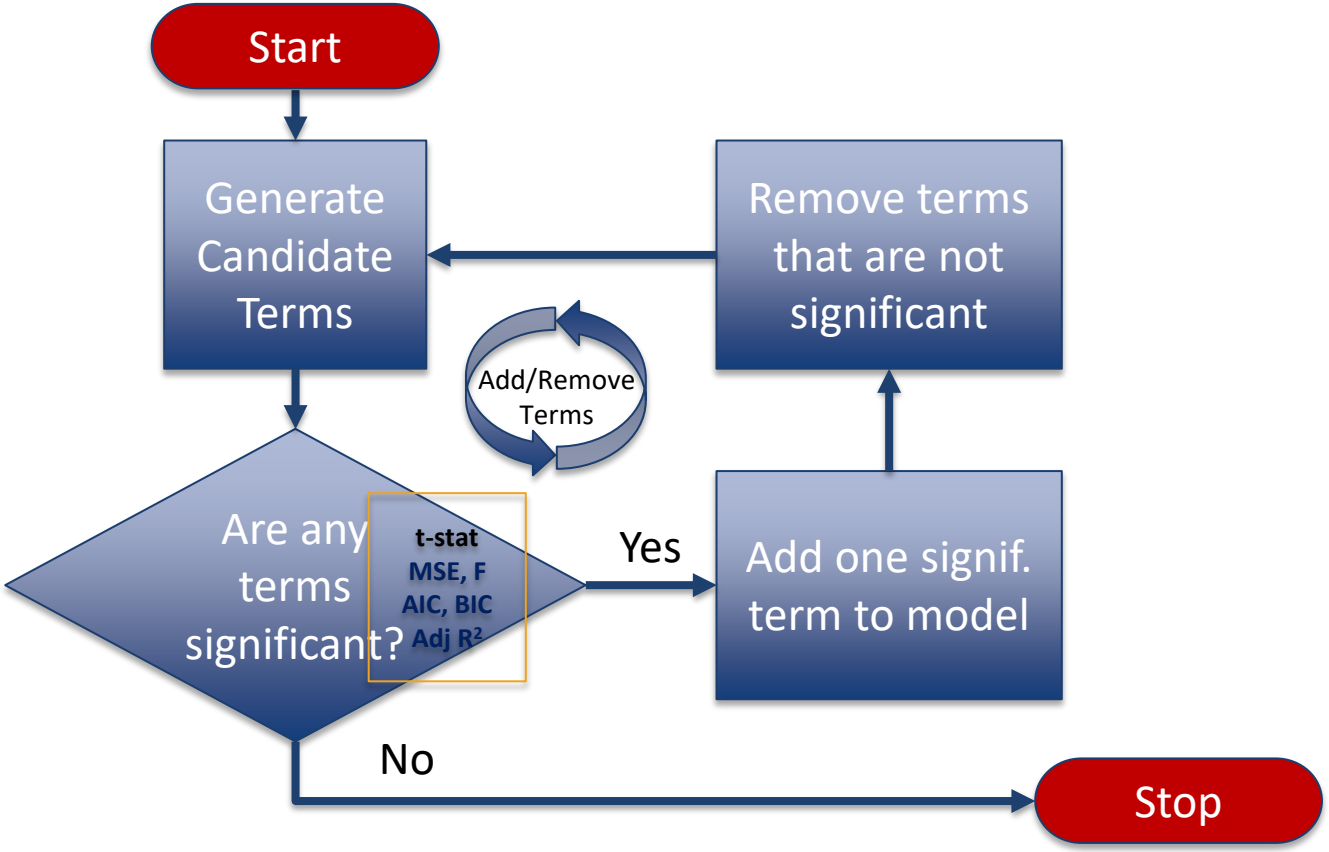
$$F = \frac{MSR}{MSE}$$

"Signal-to-noise ratio"

$$Probability\ of\ a\ larger\ value\ of\ F\ occurring\ by\ chance: = p(F, n_p, df)$$

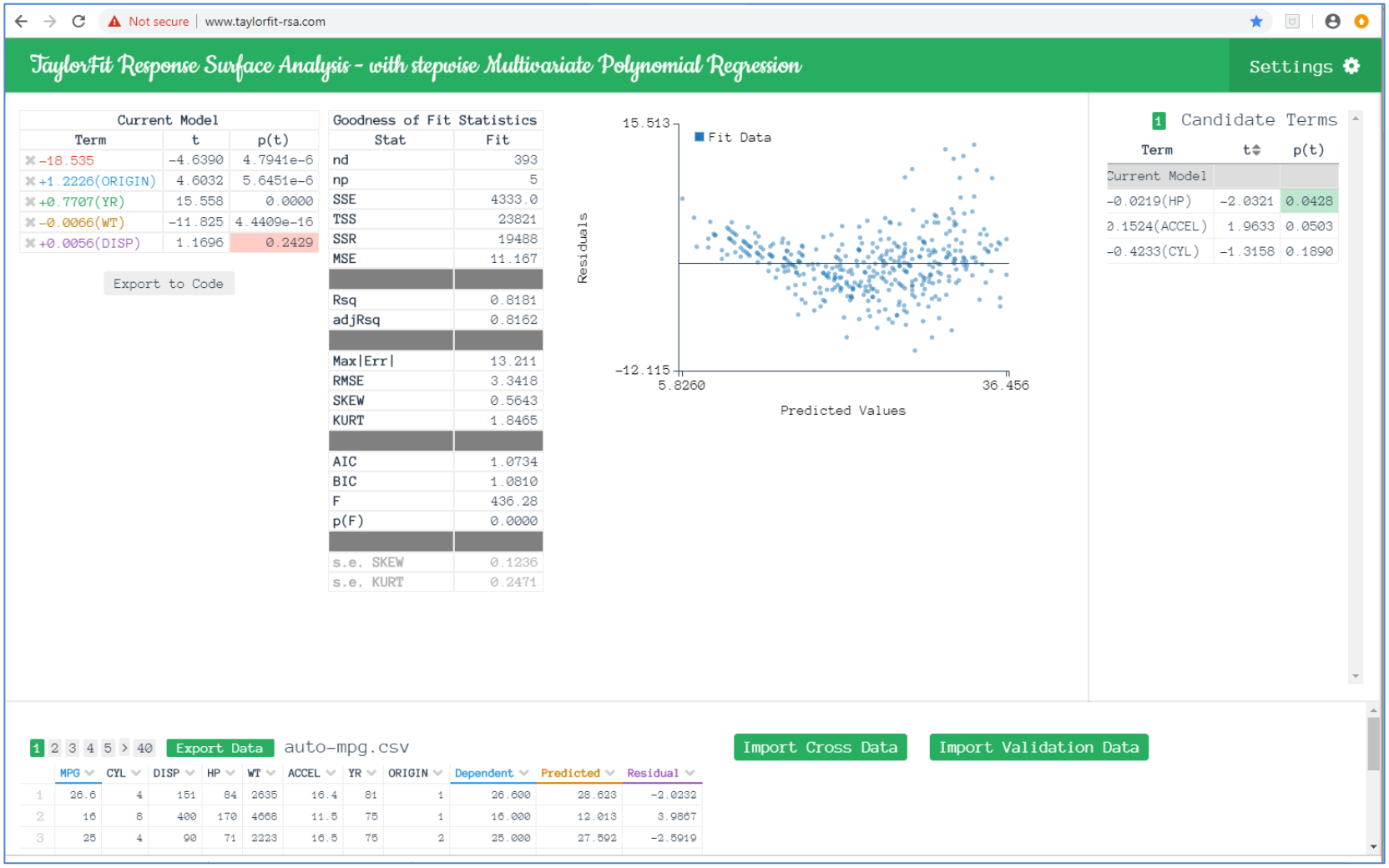
$$F = \frac{R^2_{adj}}{1 - R^2_{adj}} \cdot \frac{df}{n_p}$$

How to make models concise:
Stepwise Regression for MLR

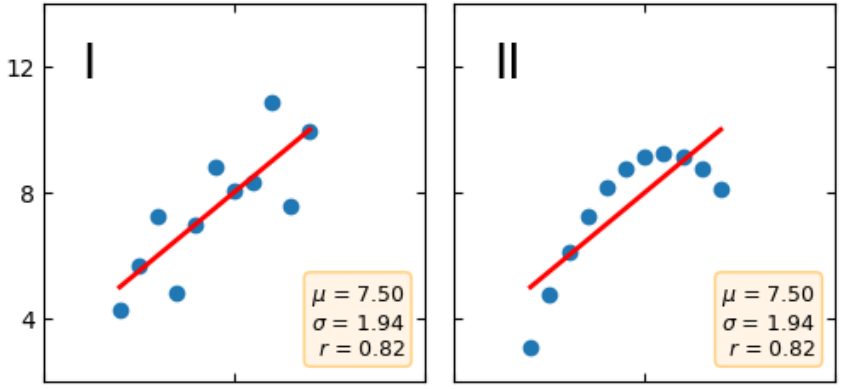


Demonstration

MLR with TaylorFit



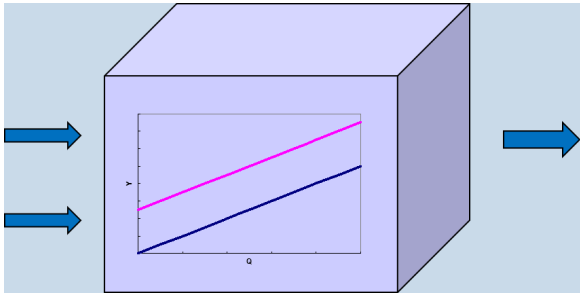
Model Specification Bias



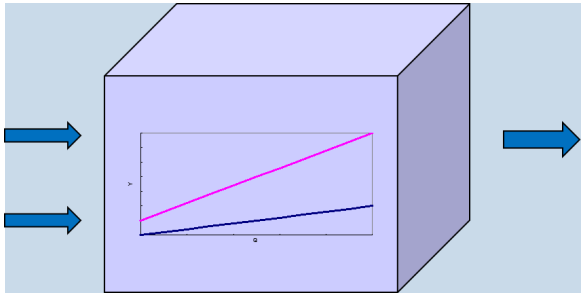
Both have the same mean, standard deviation and R^2

https://matplotlib.org/3.2.1/gallery/specialty_plots/anscombe.html

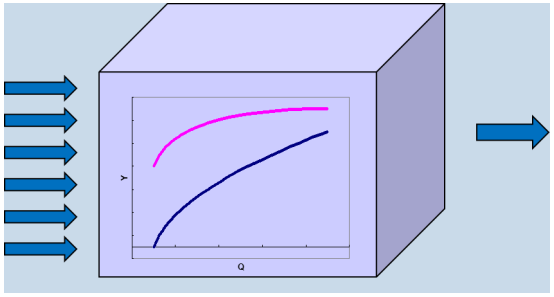
Multivariate Polynomial Regression Response Surface Analysis



Multilinear Regression



Interactions



Multivariate Polynomial (including ratios)

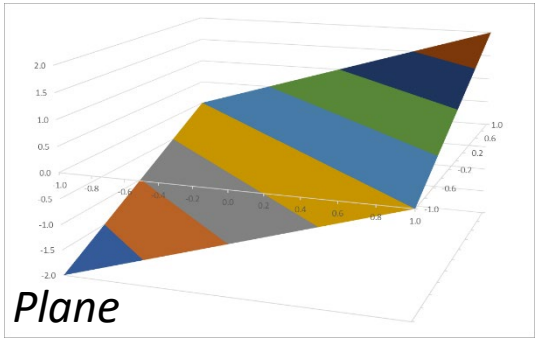
Model: $Z = a_0 + a_1 \cdot X + a_2 \cdot Y + a_3 \cdot X \cdot Y + a_4 \cdot X^2 \cdot Y^3 + a_5 \cdot X \cdot Y^{-1}$

Sensitivity: $\frac{\partial Z}{\partial X} = a_1 + a_3 \cdot Y + 2\, a_4 \cdot X \cdot Y^3 + a_5 \cdot Y^{-1}$

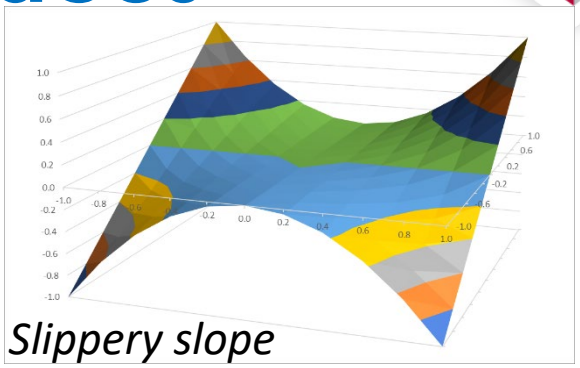
If you do not consider nonlinear relationships such as these, ***and they exist in the data***, <u>then the model will be biased</u>

Polynomial Response Surfaces

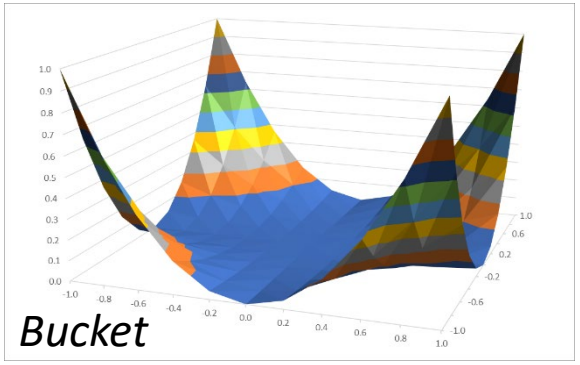
$$Z = X + Y$$



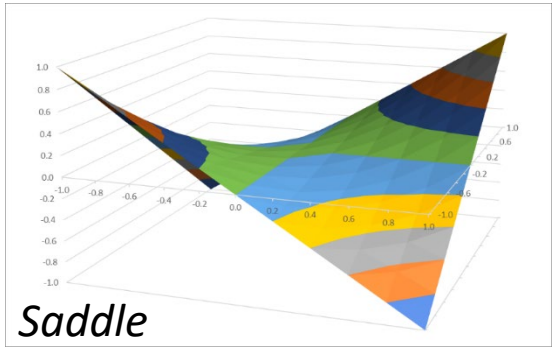
$$Z = X \cdot Y^2$$



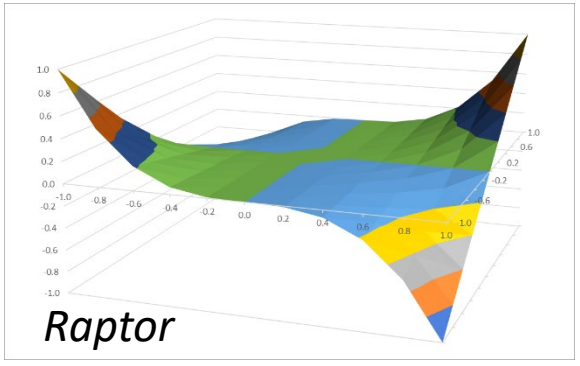
$$Z = X^2 \cdot Y^2$$



$$Z = X \cdot Y$$



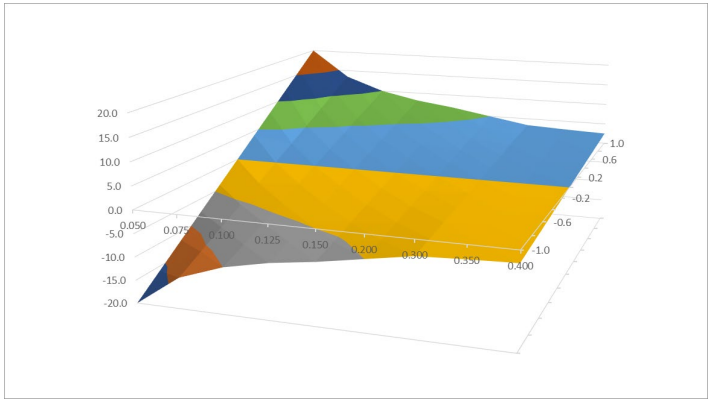
$$Z = X \cdot Y^3$$



Response Surfaces Involving Ratios

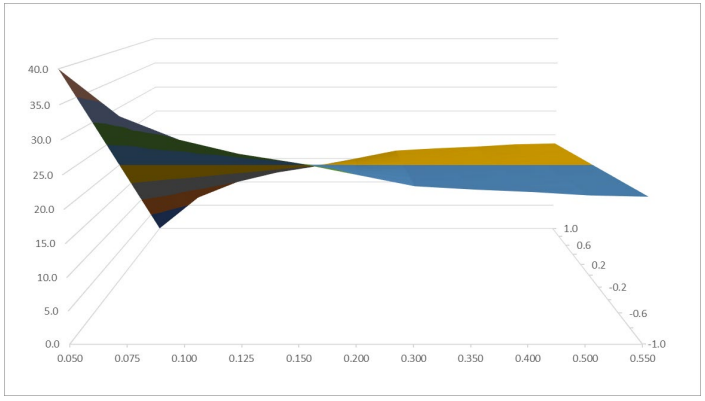
Simple ratio

$$Z = X \cdot Y^{-1}$$



Saturation

$$Z = a - X \cdot Y^{-1}$$



Example Multivariate Polynomial Model

$$Y = a_0 + a_1Q + a_2R + a_3S$$

$$+ a_4QR + a_5QS + a_6RS + a_7QRS$$
$$+ a_8Q^2 + a_9R^2 + a_{10}S^2$$

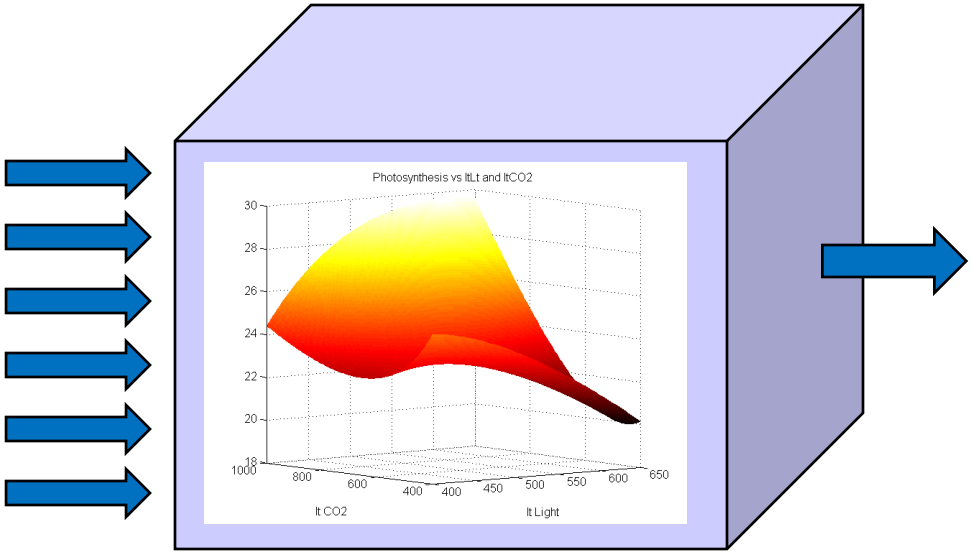
$$+ a_{11}Q^2R + a_{12}Q^2S + a_{13}Q^2R^2 + a_{14}Q^2S^2$$
$$+ a_{15}R^2S + a_{16}R^2S^2 + a_{17}QR^2 + a_{18}QS^2 + a_{19}RS^2$$

$$+ a_{20}Q^2RS + a_{21}Q^2R^2S + a_{22}Q^2RS^2 + a_{23}QR^2S^2$$
$$+ a_{24}QR^2S + a_{25}QRS^2 + a_{26}Q^2R^2S^2$$

We need a way to limit model complexity

- **STEP-WISE REGRESSION**

www.TaylorFit-RSA.com



- Accurate
- Transparent
- Transportable
- Unbiased
- Tractable
- Resistant to overfitting

Another way to ensure conciseness: Cross-validation

- Dual criteria for adding terms:
  - $p(t_{stat}) \leq \alpha$
  - Selected **GoF statistic** *for cross-validation file* associated with the candidate term improved over current model

Final Validation – The Gold Standard for Modeling

- Reserve a third partition of the dataset, called the **validation dataset**

Multivariate Polynomial Regression

TaylorFit Response Surface Analysis - with stepwise Multivariate Polynomial Regression

Settings

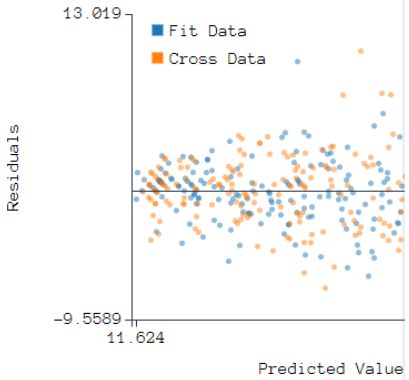
Current Model

Term	t	p(t)
-886.50	-4.2943	2.7922e-5
+6.5598(YR)	4.9124	1.9351e-6
-7.8022e-5(WT)(YR)	-2.9289	0.0038
-0.0668(HP)(ORIGIN)	-5.0127	1.2248e-6
+1.6814e-5(HP)(WT)	3.5751	4.4399e-4
+0.0028(WT)(ORIGIN)	5.6056	7.2234e-8
+30896$(YR)^{-1}$	3.9927	9.3291e-5
+2.9060e+6$(WT)^{-1}(YR)^{-1}$	3.7324	2.5050e-4

Export to Code

Goodness of Fit Statistics

Stat	Fit	Cross
nd	198	195
np	8	8
SSE	1572.9	1405.2
TSS	11960	11861
SSR	10387	10455
MSE	8.2782	7.5143
Rsq	0.8685	0.8815
adjRsq	0.8636	0.8771
Max|Err|	11.137	10.309
RMSE	2.8772	2.7412
SKEW	0.8535	0.3129
XKURT	2.4853	1.5959
AIC	0.9987	0.9579
BIC	1.0107	0.9698
F	179.25	198.77
p(F)	0.0000	0.0000
s.e. SKEW	0.1741	0.1754
s.e. XKURT	0.3482	0.3508



1 2 3 4 5 › 21 **Candidate Terms**

Term	MSE	t	p(t)
Current Model	7.5143		
-0.0032(HP)(ACCEL)	7.4427	-2.3533	0.0196
-0.1546(ACCEL)(ORIGIN)$^{-1}$	7.4444	-1.3104	0.1916
0.0174(WT)(ACCEL)$^{-1}$	7.4485	1.7873	0.0755
0.5345(ACCEL)$^{-1}$(YR)	7.4522	1.3044	0.1937
24.284(ACCEL)$^{-1}$(ORIGIN)$^{-1}$	7.4529	0.8024	0.4233
0.1944(HP)(ACCEL)$^{-1}$	7.4536	0.8871	0.3761
47.006(ACCEL)$^{-1}$	7.4552	1.5270	0.1284
0.0058(ACCEL)$^{-1}$(YR)^{2}	7.4574	1.0732	0.2846
6.0625e-6(WT)^{2}(ACCEL)$^{-1}$	7.4583	2.4331	0.0159
-0.0049(ACCEL)^{2}(ORIGIN)$^{-1}$	7.4621	-1.2035	0.2303

1 2 3 4 5 › 20 Export Data auto-mpg.csv

	MPG	CYL	DISP	HP	WT	ACCEL	YR	ORIGIN	Dependent	Predicted	Residual
1	26.6	4	151	84	2635	16.4	81	1	26.600	28.701	-2.1014
2	16	8	400	170	4668	11.5	75	1	16.000	13.424	2.5765
3	25	4	90	71	2223	16.5	75	2	25.000	27.423	-2.4228
4	18.1	6	258	120	3410	15.1	78	1	18.100	19.818	-1.7175

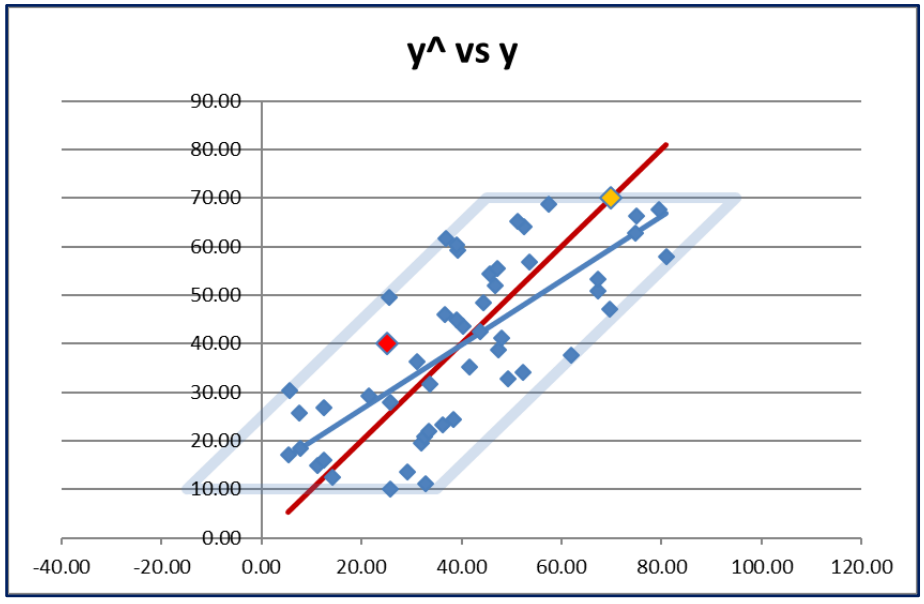
Graphical Examination of Fit

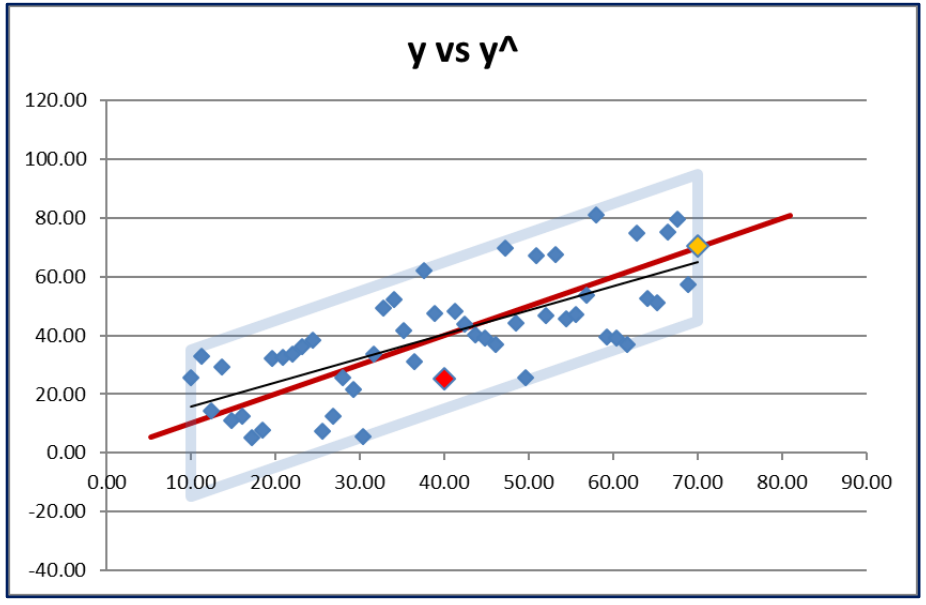
Plot predicted versus observed?

Never!

Always plot:

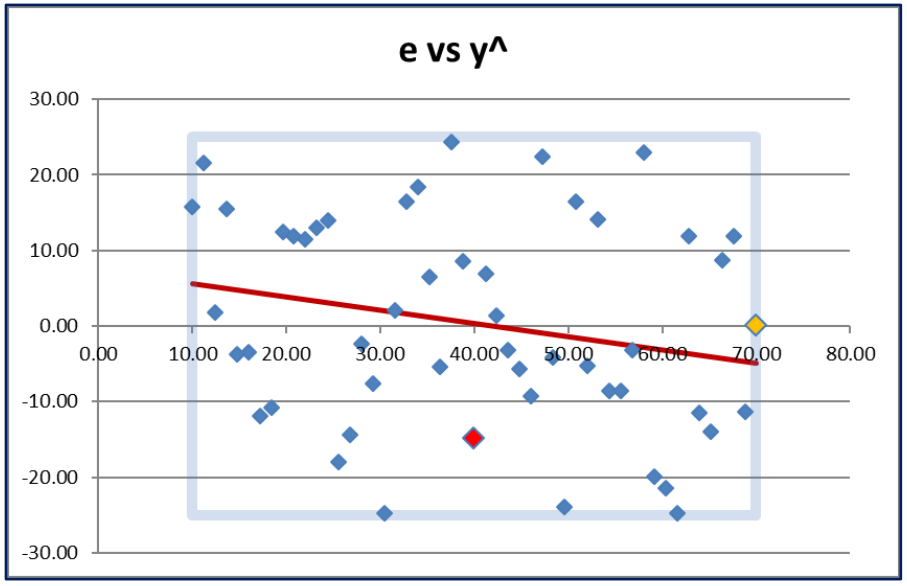
Observed versus **Predicted**

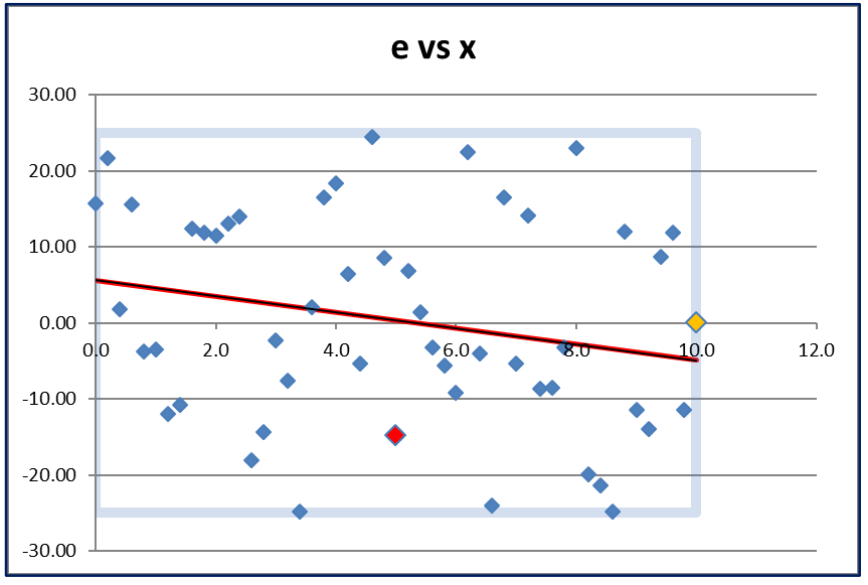




Examining Residuals

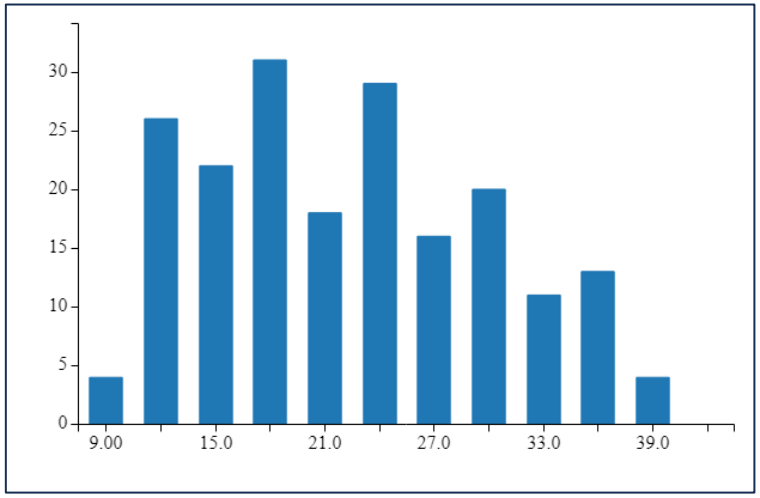
Even better: Plot residuals instead of predictions:
versus (all) data, by sequence, by time, etc.

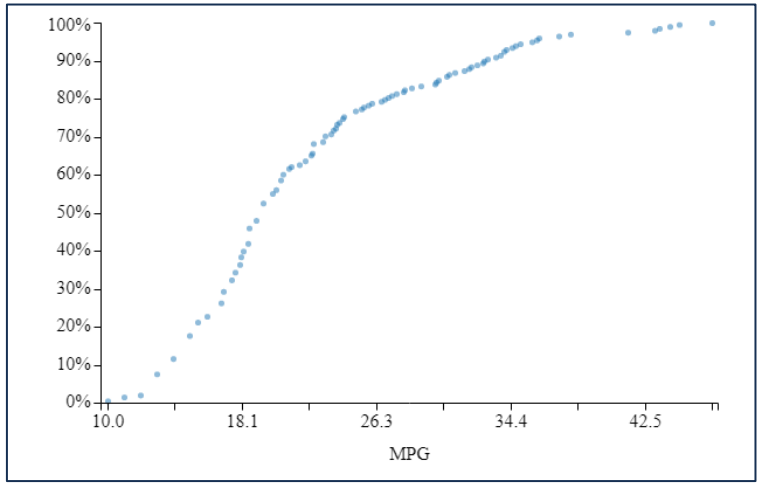


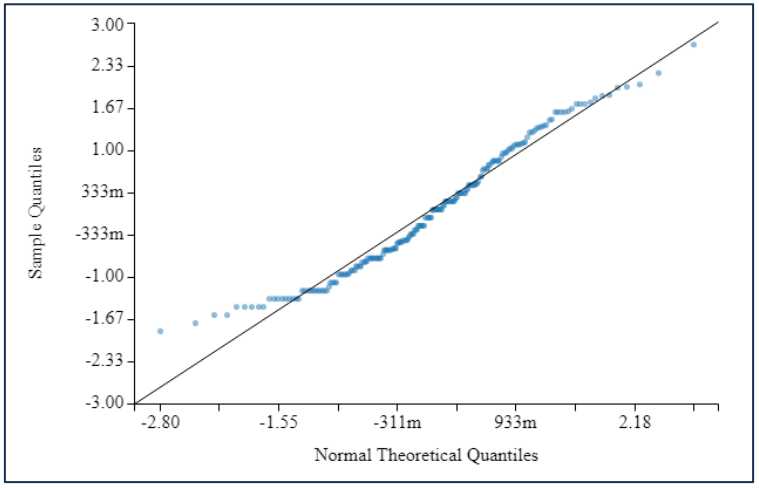


Residuals plot should appear random - no trends

Histogram, CFD, Q-Q Plot







Model Analysis

- Sensitivity
- Sensitivity distribution
- Importance ratio
- Confidence intervals

Nonlinear Local Sensitivity

Sensitivity is not constant.
So how do we represent it?

As a distribution,
based on the data:

Compute sensitivity for each datum (row)

*Mean, std. dev., **rms***
histogram, CFD, etc.

Dependence of sensitivity on units

$$MPG\left(\frac{mi}{gal}\right) = 45.6 - 0.0074 \cdot WT(lbs)$$

$$\psi_{WT} = -0.0074$$

$$MPG\left(\frac{mi}{gal}\right) = 45.6 - 0.0164 \cdot WT(kg)$$

$$\psi_{WT} = -0.0164$$

Sensitivity depends on the measurement units,
so sensitivity of different variables cannot be compared with each other

Importance ratio

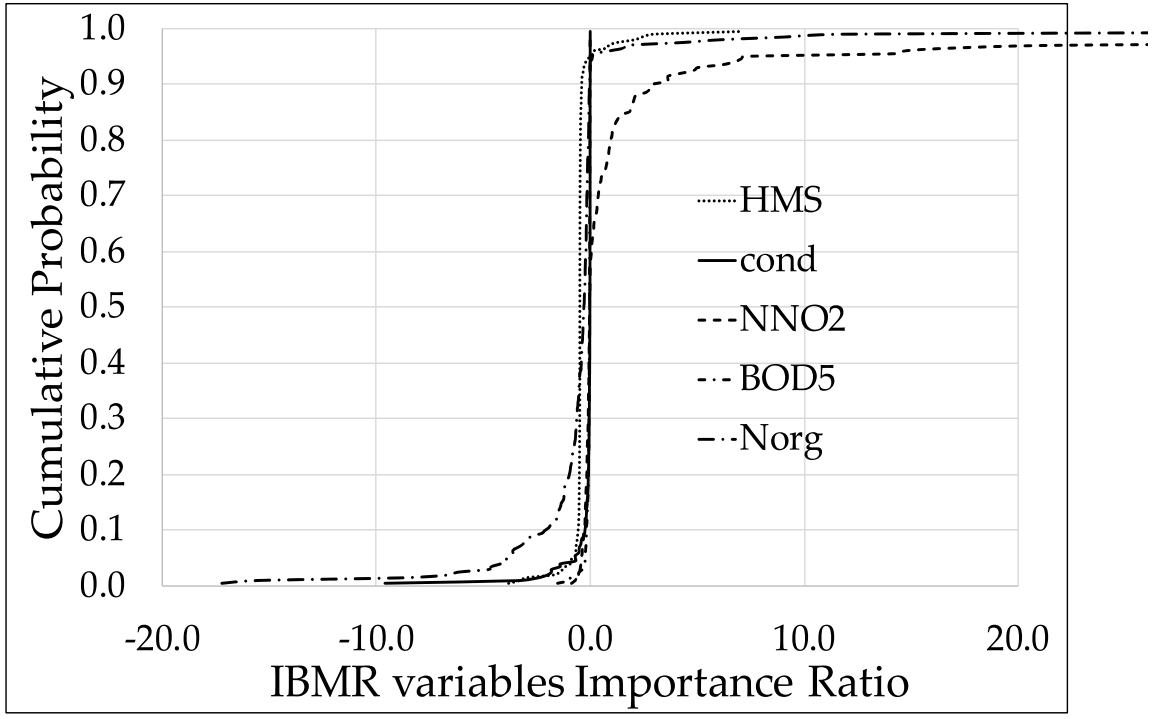
Importance ratio is a normalized sensitivity:

$$IR_{x_i} = \frac{\partial y / s.e._y}{\partial x_i / s.e._{xi}}$$

Importance ratio is dimensionless
so different I.R.'s can be compared.

Interpretation: A measure of
how much a change in x_i relative to its spread
changes y relative to its spread

Importance Ratio - Distribution



Prediction Intervals and Confidence Intervals

For Prediction: Confidence Intervals
Indicates the expected spread of the prediction

Predicted value ± C.I. (at, say, 95% confidence level)

For Observations: Prediction Intervals
Indicates the expected spread of a measured observation

Observed value ± P.I. (at, say, 95% confidence level)

Examples

- Macrophyte Indices
- Phytoplankton occurrence in the Hudson and East Rivers
- Photosynthetic productivity for NASA
- Performance of a Retail Industrial Equipment and Supply outlet

Macrophyte Index Models

Index	Equation
MIR	$3.34780 \times 10^{1} + 1.7305 \times 10^{0}(Ptot)^{-1}$
RMNI	$8.2576 \times 10^{0} - 6.2496 \times 10^{-4}(HQA)^{2}(NNO3)(Ntot)^{-1} - 1.416 \times 10^{-1}(alkal)^{-1}(Ptot)^{-1}(NNO2)^{-1} + 1.1 \times 10^{-3}(cond)(alkal)^{-1}(NNO2)^{-1} - 1.5393 \times 10^{-4}(Ptot)(NNH4)^{-1}O2^{2} + 2.2185 \times 10^{-5}(Ptot)^{-1}(NNO3)^{-1}(NNO2)^{-1}$
IBMR	$9.5335 \times 10^{0} - 2.30 \times 10^{-2}(Ptot)^{-1}(NNO2)(BOD5) + 3.226 \times 10^{-1}(Ptot)^{-1}(Norg)^{-1} - 1.4 \times 10^{-3}(alkal)(Ptot)^{-1}(Ntot)^{-1} + 1.7618 \times 10^{6}(HMS)^{-2}(cond)^{-2}(NNH4)^{-1} - 7.72 \times 10^{-2}(HMS)^{-2}(NNO2)^{-2}(Norg)^{-3}$
D	$6.806 \times 10^{-1} - 3.5578 \times 10^{-6}(HQA)^{-1}(HMS)^{2}(O2)^{2} - 8.8749 \times 10^{-6}(PPO4)^{-2}(NNH4)^{-1}(BOD5)^{-2} - 3.88 \times 10^{-2}(HMS)^{-1}(NNO3)^{-1}(BOD5)^{2} + 1.0894 \times 10^{-5}\ (HQA)^{-2}(cond)^{2}(NNO3)^{-1}$
N	$3.2233 \times 10^{1} - 9.30 \times 10^{-2}(HMS) - 9.4650 \times 10^{1}(pH)(alkal)^{-1} - 3.438 \times 10^{-1}(HQA)^{-1}(alkal) - 3.1979 \times 10^{2}(cond)^{-1}(BOD5) - 1.9307 \times 10^{0}(HMS)^{-1}(NNO3)(NNO2)^{-1} + 1.2670 \times 10^{-4}(NNO2)^{-1}(NNH4)^{-1}(Ntot) - 9.64 \times 10^{-2}(cond)(NNO2)(O2)^{-1}$

Indices of trophic and ecological status of the rivers:

Macrophyte Index for Rivers (MIR)

River Macrophyte Nutrient Index (RMNI)

Macrophyte Biological Index for Rivers (IBMR)

Biological diversity indices:

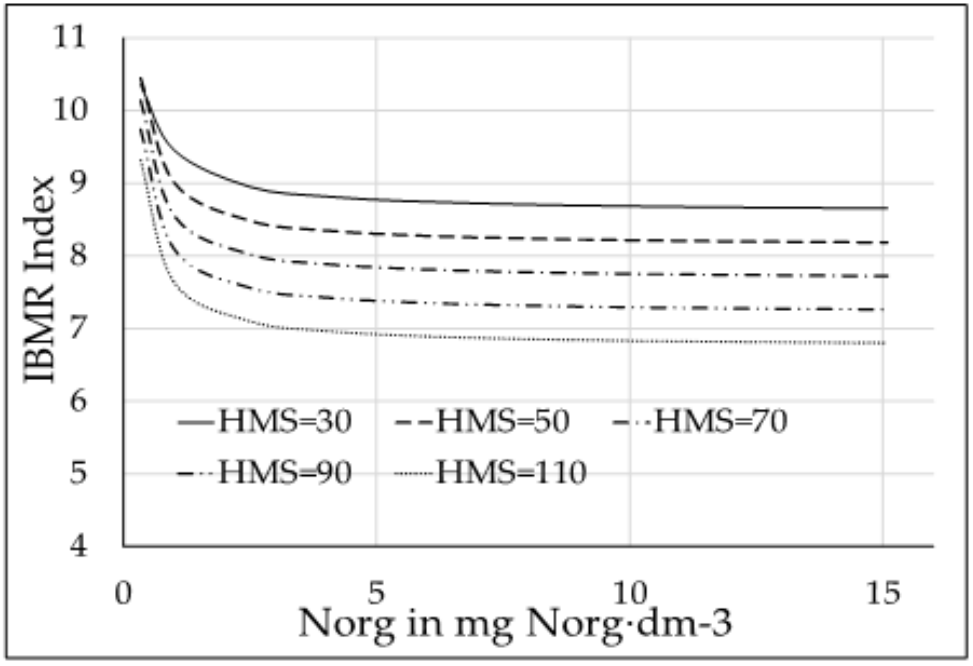
Simpson index (D)

Species richness (N)

Vishwa Shah, Sarath Chandra K. Jagupilla *, David A. Vaccari, Daniel Gebler (2021). Non-Linear Visualization and Importance Ratio Analysis of Multivariate Polynomial Regression Ecological Models based on River Hydromorphology and Water Quality. Section: Ecohydrology, *Water* 2021, 13, 2708. https://doi.org/10.3390/w13192708.

Nonlinear Behavior of IBMR

$$
\begin{aligned}
IBMR = \; & 9.5335 \times 10^{0} \\
& -2.30 \times 10^{-2}(Ptot)^{-1}(NNO2)(BOD5) \\
& +3.226 \times 10^{-1}(Ptot)^{-1}(Norg)^{-1} \\
& -1.4 \times 10^{-3}(alkal)(Ptot)^{-1}(Ntot)^{-1} \\
& +1.7618 \times 10^{6}(HMS)^{-2}(cond)^{-2}(NNH4)^{-1} \\
& -7.72 \times 10^{-2}(HMS)^{-2}(NNO2)^{-2}(Norg)^{-3}
\end{aligned}
$$



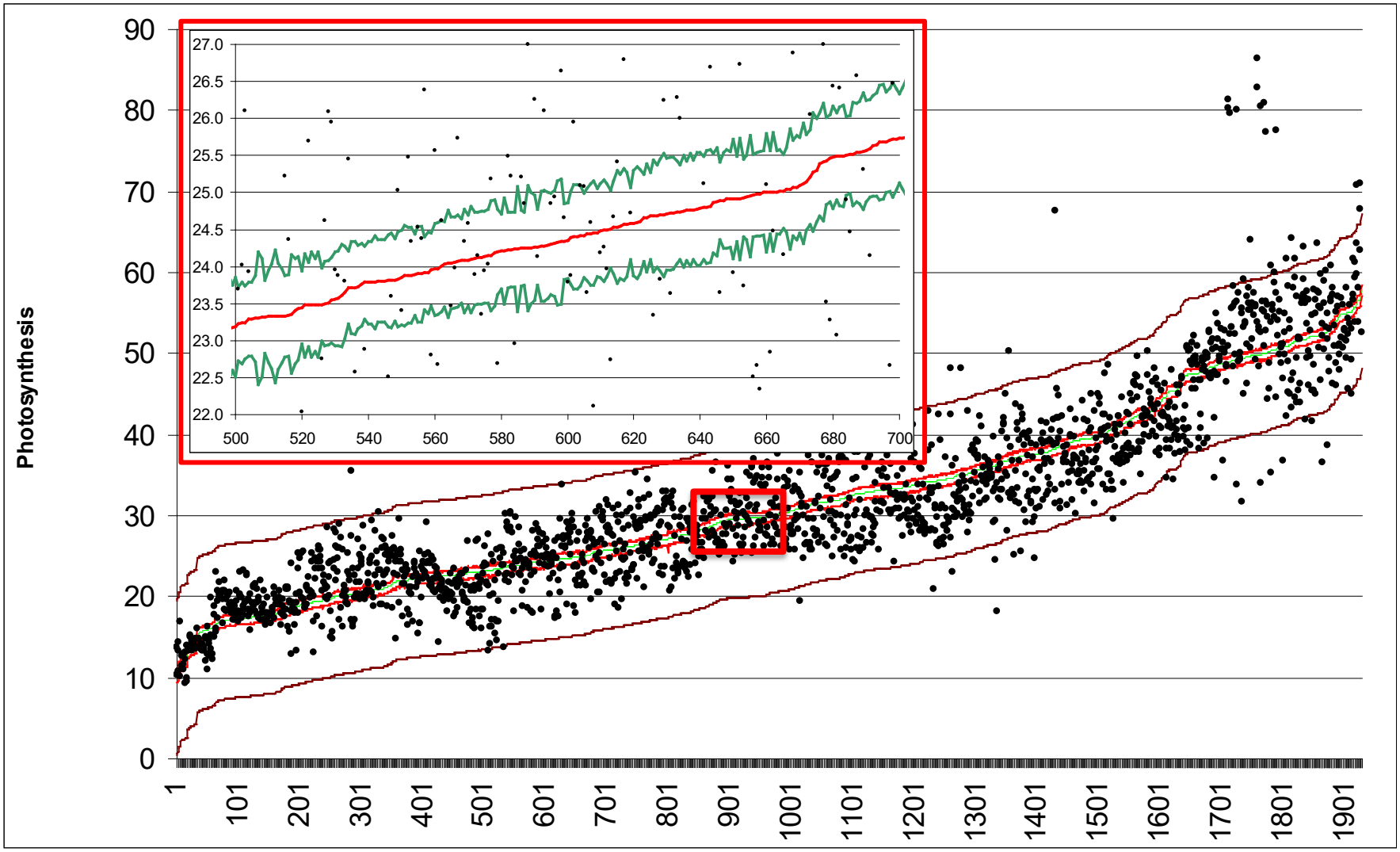
IBMR vs organic nitrogen with river morphology as a parameter.
(HMS – River Hydromorphological Index)

GoF Performance of MPR vs. ANNs

	Type of Model	Validation R^2	Degrees of Freedom (df) for Error	Mean Square Error (MSE)	F-Stat	p(F)
MIR	MPR	0.58	12	10.856	1.11	0.373
	ANN	0.702	52	9.790		
RMNI	MPR	0.65	9	0.048	1.00	0.452
	ANN	0.715	52	0.050		
IBMR	MPR	0.47	9	0.364	0.88	0.551
	ANN	0.532	52	0.411		
D	MPR	0.237	8	0.008	1.00	0.447
	ANN	0.284	52	0.009		
N	MPR	0.33	11	8.392	0.90	0.544
	ANN	0.415	52	9.288		

$p(F) > 0.05$ means the difference between MPR and ANN model accuracy was not statistically significant

Experimental Photosynthesis Data, Prediction, Confidence Intervals for Observations and Predictions

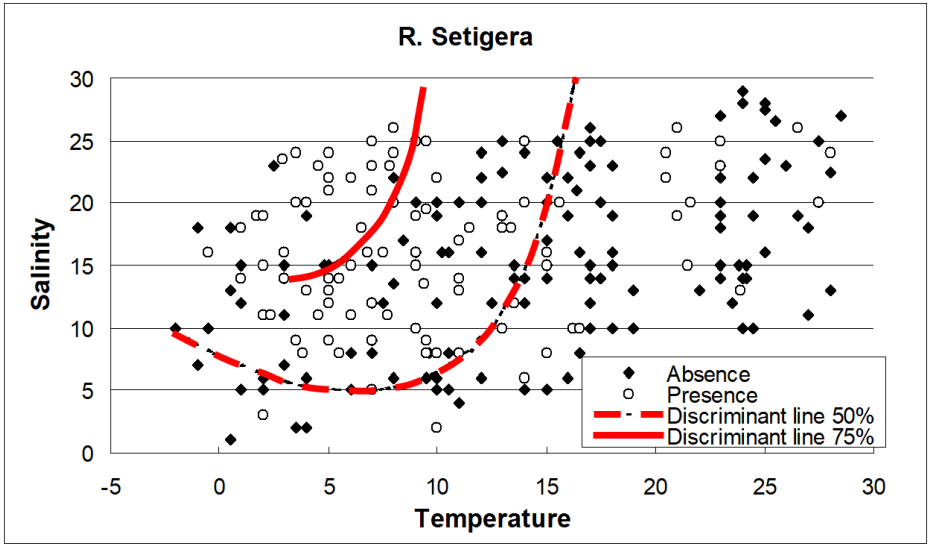


Classification model for presence of phytoplankton

- Presence or absence of 3 phytoplankton species (coded variable)

- Salinity
- Water temperature
- Dissolved oxygen
- pH
- Secchi disk depth
- Percent cloud cover
- Tidal stage
- Wind

$$y = 1.17 \cdot 10^{-2} \cdot pH^2 - 9.74 \cdot 10^{-3} \cdot T \cdot DO + 8.8 \cdot 10^{-4} \cdot T \cdot DO^2 + 2.37 \cdot 10^{-4} \cdot S \cdot DO^2 + 5.3 \cdot 10^{-4} \cdot pH \cdot DO^2 - 0.34$$



Z. Wang, D.A. Vaccari, M. Levandowsky. Multivariate Polynomial Modeling of Phytoplankton in the Lower Hudson River. Platform presentation, American Society of Limnology and Oceanography, summer meeting, Savannah Georgia, 2004.

Performance of Retail Industrial Sales Outlet

$$GM = 3.72 + 0.56 \cdot SE - \frac{1}{15.5 \cdot M \cdot Y} + \frac{93.45}{S \cdot C} + \frac{1}{81.7 \cdot Y \cdot W} + \frac{Q}{69.2}$$

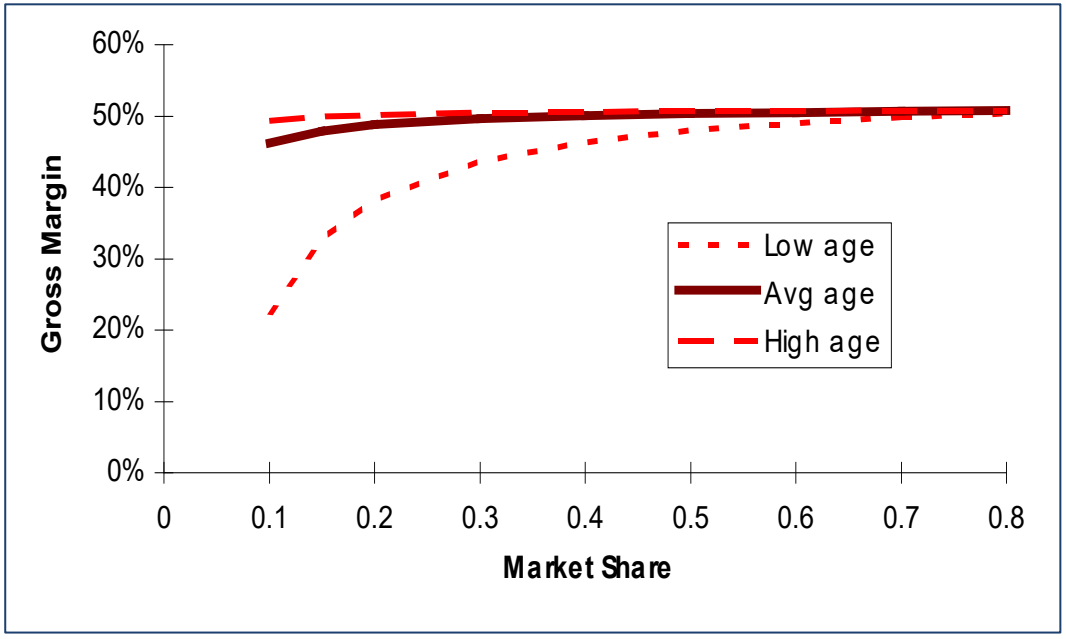
$R^2 = 0.82$ (82%)

Variables used:

- Supply/equipment ratio
- Market share
- Years at location
- Sales
- Competition intensity
- Walk-in/delivery ratio
- Quality

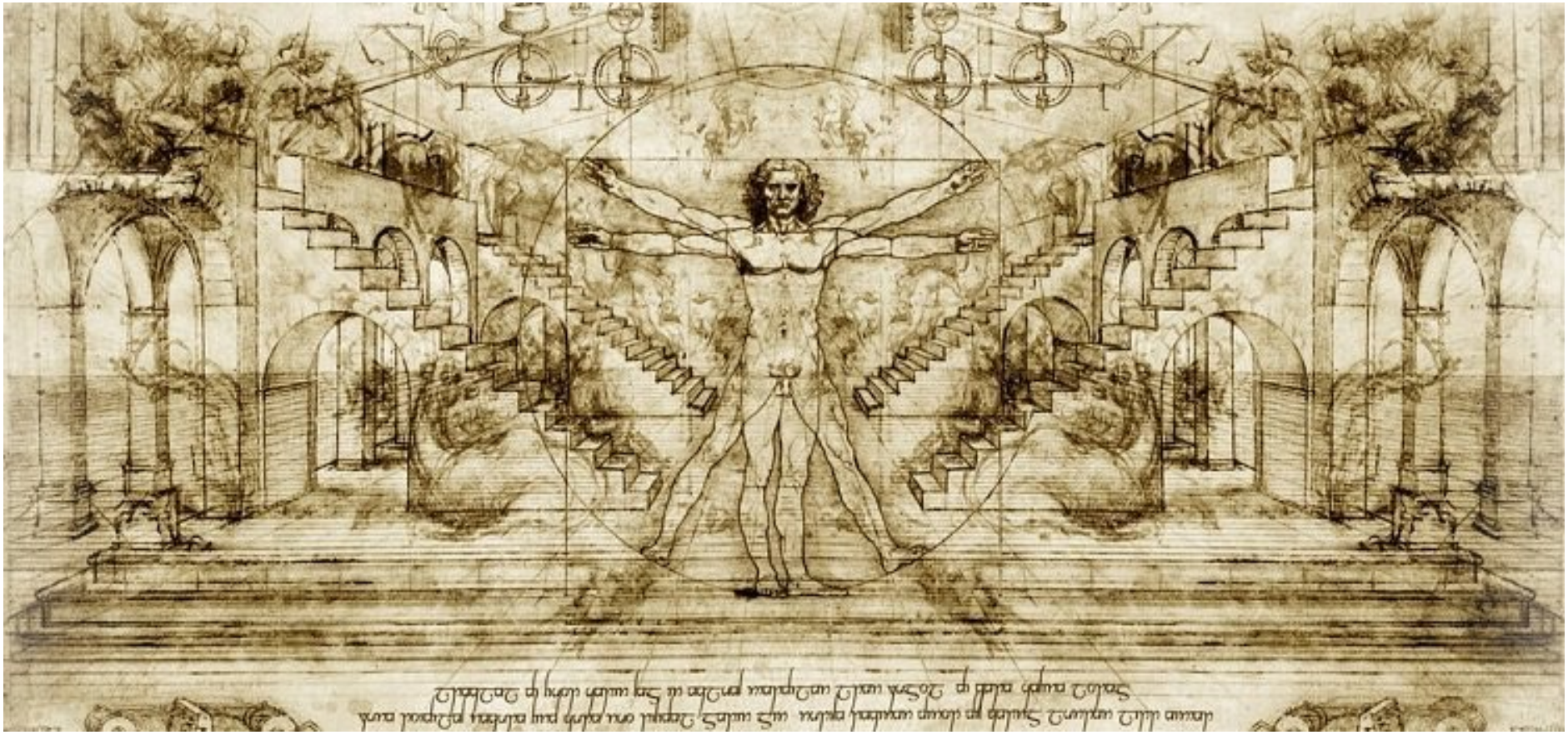
Variables not significant:

- Industrial concentration
- Rural/Urban location
- Highway visibility
- # of staff
- Average years of service
- # of salespersons



Effect of *Market Share* with *Years at Location* as a parameter

Modeling is Art as well as Science



The Vitruvian Man – Leonardo Da Vinci

https://www.leonardodavinci.net/

Thank you

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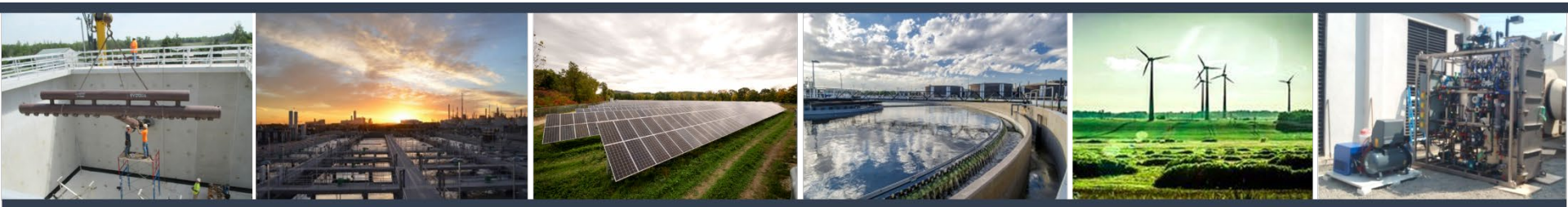

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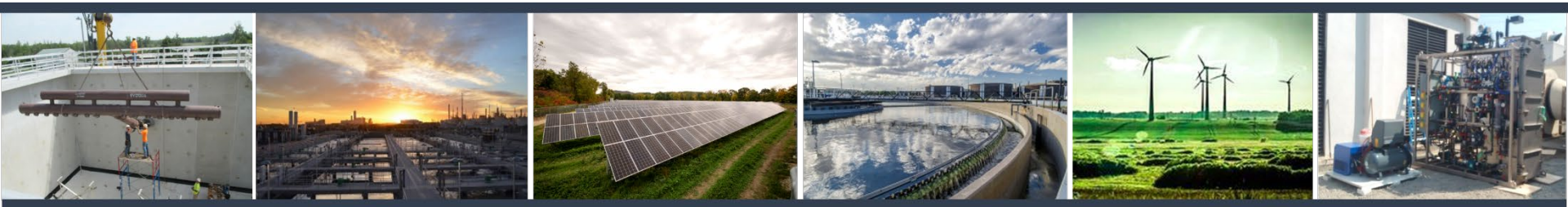


Bibliography

Users' Manual for *TaylorFit* Response Surface Analysis Using Multivariate Polynomial Regression. (2019) www.TaylorFit-RSA.com.

Non-time-series:

Vaccari, D.A., Nonlinear Analysis of Retail Performance, *Proceedings of the IEEE/IAFE Conference on Computational Intelligence for Financial Engineering* (CIFEr), pp252-258, New York, NY, March 24-26, 1996.

Vaccari, D.A. and J. Levri, "Multivariable Empirical Modeling of ALS Systems Using Polynomials," *Life Support and Biosphere Science*, vol. 6 pp. 265-271, (1999).

Jagupilla, S.J.K., D.A. Vaccari; R.I. Hires, "Multivariate Polynomial Time-Series Models and Importance Ratios to Identify Fecal Coliform Sources," *ASCE Journal of Environmental Engineering*, v136, n7, pp657-665 (2010).

V. Shah, S.C. K. Jagupilla *, D. A. Vaccari, D. Gebler (2021). Non-Linear Visualization and Importance Ratio Analysis of Multivariate Polynomial Regression Ecological Models based on River Hydromorphology and Water Quality. Section: Ecohydrology, *Water* 2021, 13, 2708. https://doi.org/10.3390/w13192708.

Z. Wang, D.A. Vaccari, M. Levandowsky. Multivariate Polynomial Modeling of Phytoplankton in the Lower Hudson River. American Society of Limnology and Oceanography, summer meeting, Savannah Georgia, 2004.

Time-series:

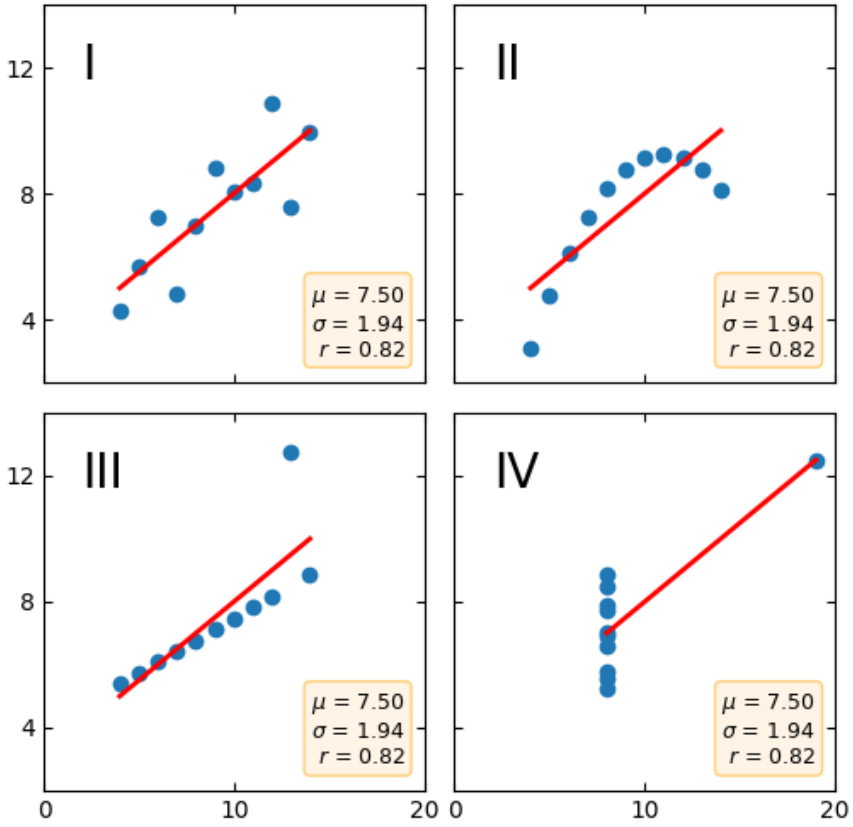
Vaccari, D. A. and H.K. Wang, "Multivariate polynomial regression for identification of chaotic time series," *Mathematical and Computer Modelling of Dynamical Systems*, v13, n4, pp395–412 (2007).

Watson, R., Nieradka, B. and Vaccari, D. A. (2017), Empirical Dynamic Material Flow Model for Tungsten in the USA. *Journal of Industrial Ecology*. doi:10.1111/jiec.12555.

Empirical Modeling Pitfalls

- Overfitting
- Spurious correlation
- Polynomial wiggle
- Outliers
- Influential points
- Multicollinearity
- Nonlinear bias
- Explosive behavior
- Heteroscedasticity

Anscombe's Quartet



All have the same
mean, standard deviation and R^2

I – Typical regression
II – Nonlinear
III – Outlier
IV – Influential point

Shows the importance of graphical examination of the data and not just relying on statistical measures

https://matplotlib.org/3.2.1/gallery/specialty_plots/anscombe.html