Multivariate Modeling: Multivariate

Lecture outline . . .

Multivariate Analysis

Joints and Conditionals

Feature Selection

Multivariate Estimation

Introduction

Fundamental Concepts

Probability

Data Prep / Analytics

Spatial Continuity / Prediction

Multivariate Modeling

Uncertainty Modeling

Machine Learning

Instructor: Michael Pyrcz, the University of Texas at Austin

Multivariate Modeling: Multivariate

Lecture outline . . .

Multivariate Analysis

Introduction

Fundamental Concepts

Probability

Data Prep / Analytics

Spatial Continuity / Prediction

Multivariate Modeling

Uncertainty Modeling

Machine Learning

Instructor: Michael Pyrcz, the University of Texas at Austin

Motivation for Multivariate Methods

We typically need to build reservoir models of more than one property of interest.

- Expanded by whole earh modeling, closing loops with forward models
- Expanded by unconventionals

Subsurface properties may include:

- Rock Classification: lithology, architectural elements, facies, depofacies
- Petrophyscial: porosity, directional permeability, saturuations
- Geophysical: density, p-wave and s-wave velocity
- Gemechanical: compressibility / Poisson's ratio, Yong's modulus, brittleness, stress field
- Paleo- / Time Control: fossil adundances, stratigraphic surfaces, ichnofacies, paleo-flow indicators

Curse of Dimensionality



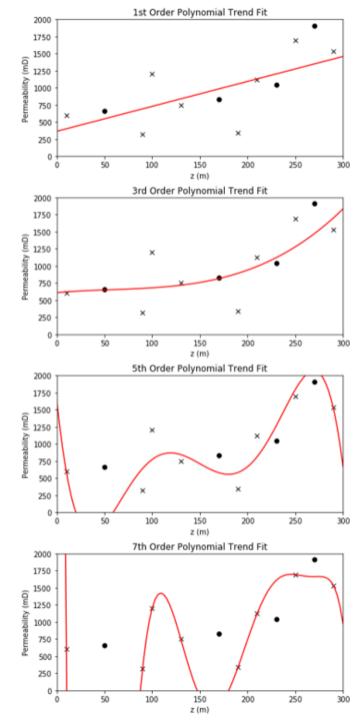
Working with more features / variables is harder!

- More difficult to visualize
- 2. More data are required to infer the joint probabilities
- 3. Less coverage
- 4. More difficult to interrogate / check the model
- 5. More likely redundant
- 6. More complicated, more likely overfit

Visualization

Consider this simple model:

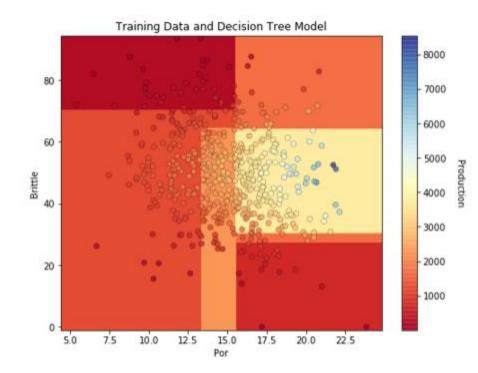
- 1 predictor feature
- 1 response feature
- How's our model performing?
 - Accuracy in training and testing
- Range of Applicability?
 - Are we extrapolating?
- Overfit
 - Is the model defendable given the data?





Consider this simple model:

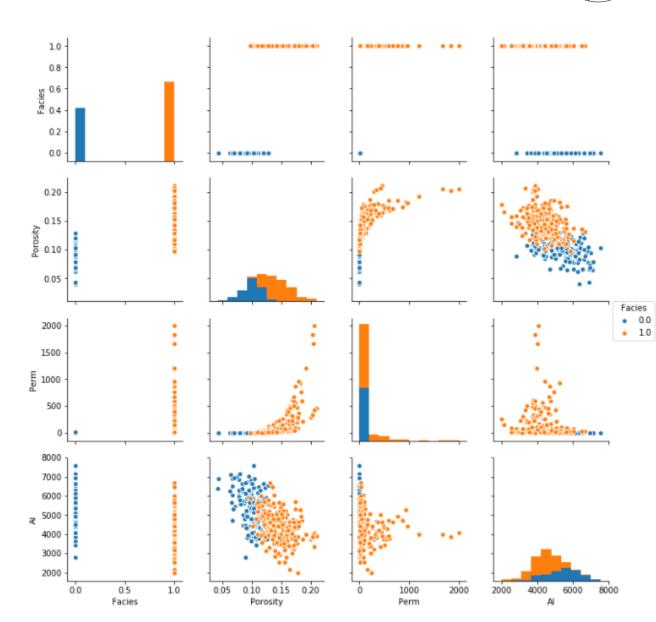
- 2 predictor features
- 1 response feature
- How's our model performing?
 - Accuracy in training and testing
- Range of Applicability?
 - Are we extrapolating?
- Overfit
 - Is the model defendable given the data?



Visualization Visualization

Consider this:

- 4 predictor features
- 1 response feature (not shown)
- What are the relationships between features?
- Are there constraints?



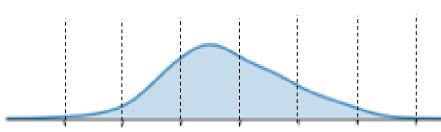
Inferring Joint Probabilities



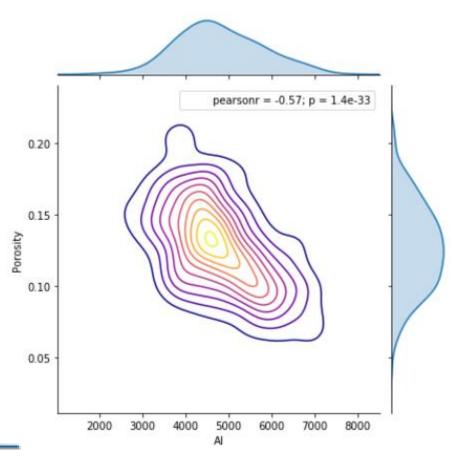
 Consider any joint probability:

$$P(X_1 \cap, ..., \cap X_m)$$
 the joint probability of $X_1, ..., X_m$

 Let's start with 1 feature (m=1)



$$P(X_1^i \le X \le X_1^{i+1}) = \frac{n(X_1^i \le X \le X_1^{i+1})}{n}$$



In each bin we are estimating a probability!

10 data in each bin = 80 data?

Inferring Joint Probabilities



 Consider any joint probability:

$$P(X_1 \cap, ..., \cap X_m)$$
 the joint probability of $X_1, ..., X_m$

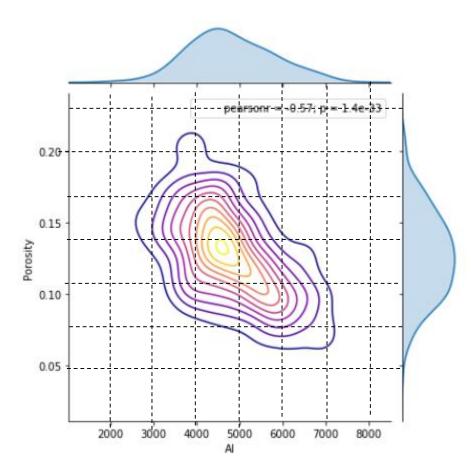
 Now move to 2 features (m=2)

$$P(X_1^i \le X \le X_1^{i+1}, X_2^j \le X \le X_2^{j+1})$$

$$= \frac{n(X_1^i \le X \le X_1^{i+1}, X_2^j \le X \le X_2^{j+1})}{n}$$

$$n = Data/Bin \cdot Bins^m$$

This is optimistic, as it assumes uniform sampling



In each bin we are estimating a probability!

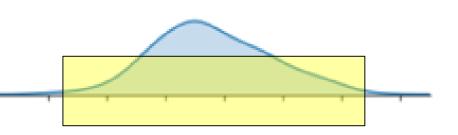
10 data in each bin = 640 data?

Coverage



Consider coverage:

- The range of the sample values
- The fraction of the possible solution space that is sampled.
- Let's return to 1 feature, and assume 80% coverage!
- That's pretty good right?



Coverage



Consider coverage:

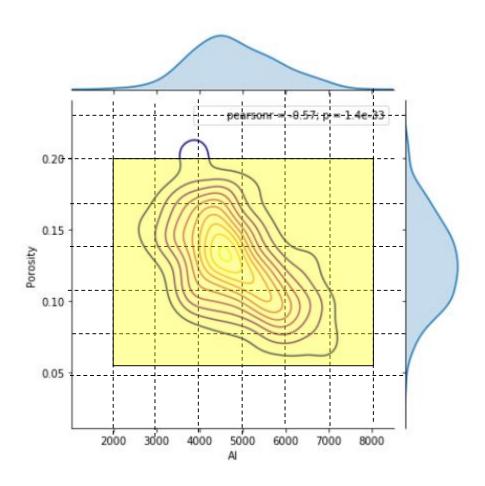
- Now let's move to 2 features, each with 80% coverage
- How much of the solution space is covered?

$$0.8^D$$
, $e.g. 0.8^2 = 0.64$

Even with exponential increase in number of data:

$$n = Data/Bin \cdot Bins^m$$

coverage is decreasing as we increase the number of features!

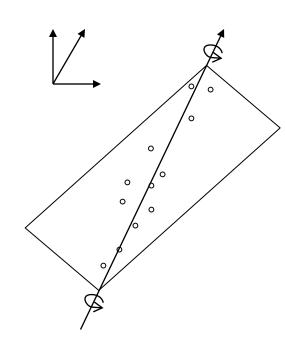


Multicollinearity Feature Redundancy

"the existence of such a high degree of correlation between supposedly independent variables being used to estimate a dependent variable that the contribution of each independent variable to variation in the dependent variable cannot be determined"

- Merriam-Webster Online Dictionary

"In statistics, multicollinearity (also collinearity) is a phenomenon in which one predictor variable in a multiple regression model can be linearly predicted from the others with a substantial degree of accuracy."

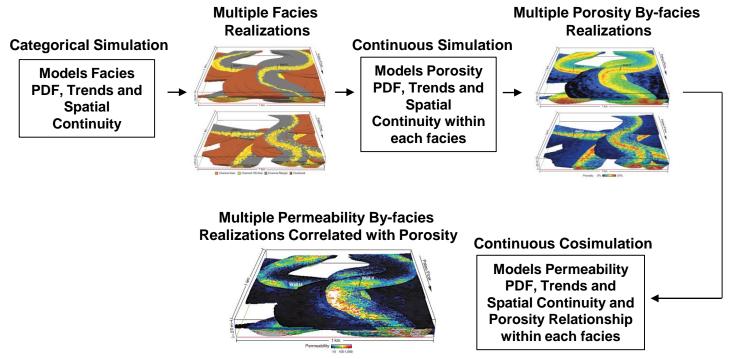


It is like fitting a plane to a line!

Motivation for Multivariate Methods

A Confession:

- Standard geostatistical workflows are bivariate at most
 - » e.g. simulate permeability conditional to porosity



Note: only had 1 realization on hand (should be two in figure).

Motivation for Multivariate Methods

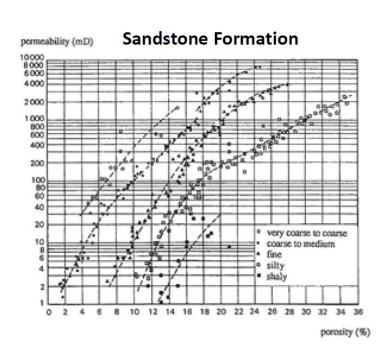
Emerging Multivariate Methods Include:

 Transforms – remove correlations and then model with independent variables and then back-transform to restore correlation (e.g. step-wise conditional transform).

This is beyond the scope of this course.

Bivariate StatisticsWhat is Bivariate Analysis?

- Bivariate Analysis: Understand and Quantify the relationship between two variables
 - Example: Relationship between porosity and permeability
 - How can we use this relationship?



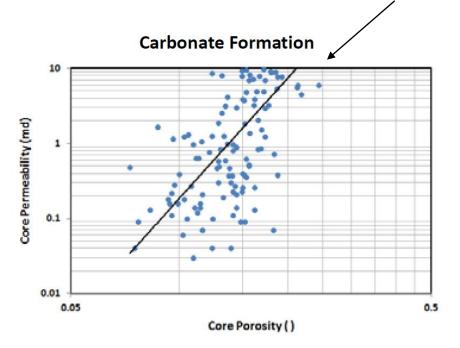
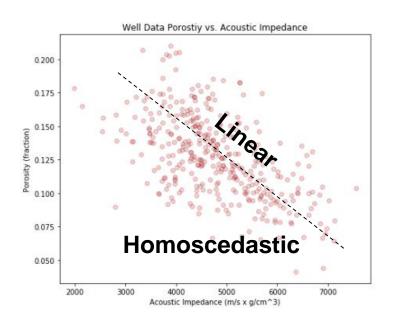


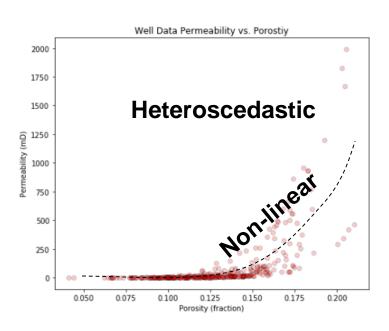
Figure from Peters, E. J., 2012, Advanced Petrophysics.

Scatter Plot

Bivariate Statistics What is Bivariate Analysis?

Examples of bivariate structures

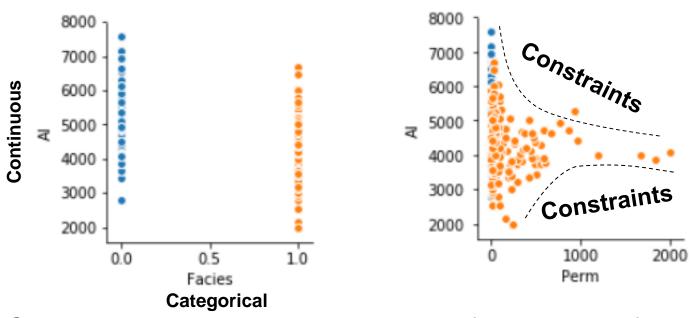




- Linear / Nonlinear shape of the conditional expectation Y | X
- Homoscedastic / Heteroscedastic conditional variance of Y | X

Bivariate Statistics What is Bivariate Analysis?

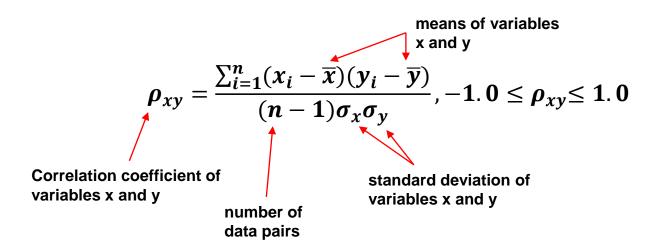
Examples of bivariate structures



- Categorical variables only have a specified number of possible outcomes, continuous takes on a range of possible outcomes.
- Constraints specific combinations of variables are not possible.

Bivariate StatisticsPearson's Correlation Coefficient

- Definition: Pearson's Product-Moment Correlation Coefficient
 - Provides a measure of the degree of linear relationship.



Correlation coefficient is a standardized covariance.

$$C_{xy} = \frac{\sum_{i=1}^{n} (x_i - \overline{x})(y_i - \overline{y})}{(n-1)}$$
 Covariance $\rho_{xy} = \frac{C_{xy}}{\sigma_x \sigma_y}$

- We can see that covariance and variance are related.
 - Replace the second term in the square with another variable.
 - Covariance:

$$C_{xy} = \frac{1}{n-1} \sum_{i=1}^{N} (x_i - \bar{x})(y_i - \bar{y})$$

A measure of how 2 variables vary together.

– Variance:

$$s^{2} = \frac{1}{n-1} \sum_{i=1}^{N} (x_{i} - \bar{x})(x_{i} - \bar{x})$$

A measure of how 1 variable varies with itself.



Spearman's Rank Correlation Coefficient

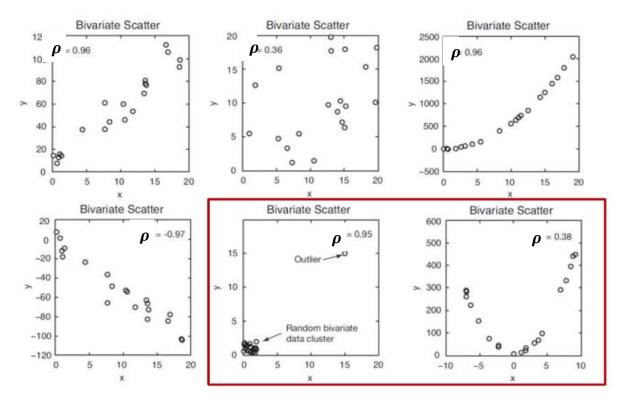
- Definition: Spearman's Rank Correlation Coefficient
 - Provides a measure of the degree of monotonic relationship.

$$\rho_{R_x,R_y} = \frac{\sum_{i=1}^n (R_{x_i} - \overline{R_x})(R_{y_i} - \overline{R_y})}{(n-1)\sigma_{R_x}\sigma_{R_y}}, -1.\ 0 \le \rho_{xy} \le 1.\ 0$$
 Rank correlation coefficient of variables x and y number of data pairs

- Rank transform, e.g. R_{x_i} , sort the data in ascending order and replace the data with the index, i = 1, ..., n.
- Spearman's rank correlation coefficient is more robust in the presence of outliers and some nonlinear features than the Pearson's correlation coefficient

Bivariate StatisticsPearson's Correlation Coefficient

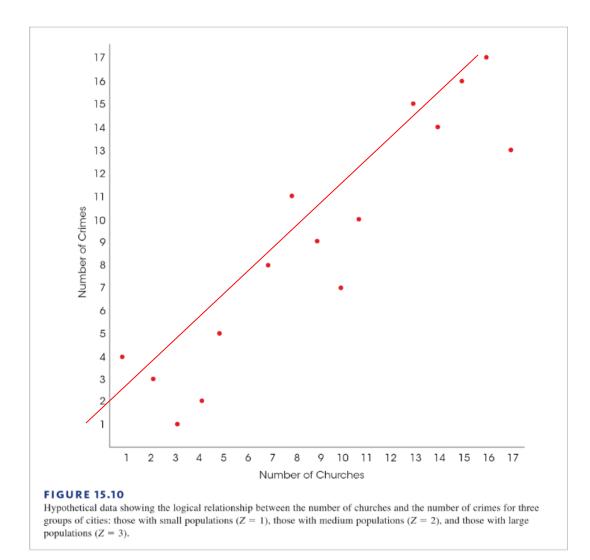
Interpreting the correlation coefficient



Is Pearson's correlation coefficient a reliable measure of correlation in these cases?

Bivariate StatisticsCorrelation and Causation

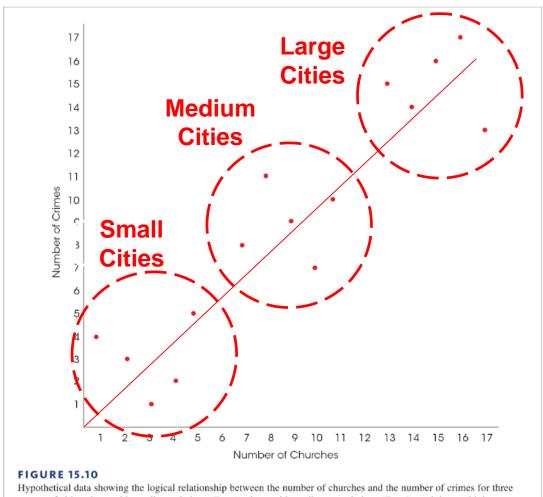
- Correlation does not imply causation!
 - We require a
 "true experiment"
 where one
 variable is
 manipulated and
 others are
 rigorously
 controlled!



Bivariate StatisticsCorrelation and Causation

The first of Good History

- Correlation does not imply causation!
 - Population was not controlled!
 - For each size of city the correlation is nearly zero.



Hypothetical data showing the logical relationship between the number of churches and the number of crimes for three groups of cities: those with small populations (Z = 1), those with medium populations (Z = 2), and those with large populations (Z = 3).

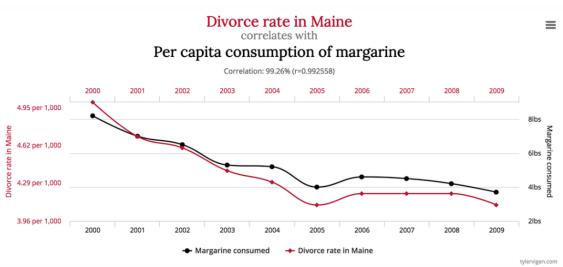
Comical Examples of Correlation and Causation



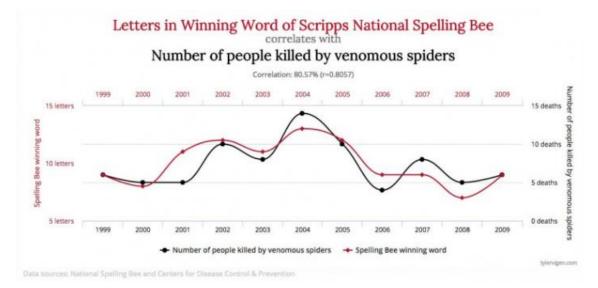
Margarine causes **divorce**? or **divorce** causes **margarine**?

Spiders killing people causes longer words in spelling bees?

or longer words in spelling bees causes venomous spiders to kill people?



ata sources: National Vital Statistics Reports and U.S. Department of Agriculture



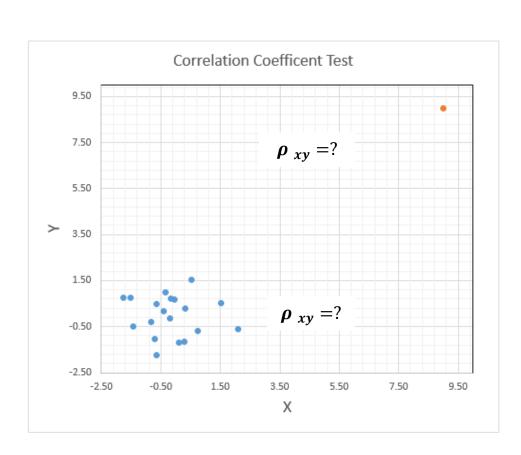
THE LIGHT OF THE PARTY OF THE P

Exercise with Pearson's Correlation Coefficient

 Task 1: Generate a random data set of x and y variables and estimate their correlation coefficient (Hint: Rand() in Excel with N[0,1]).

 Task 2: Now add any desired outlier to the data and estimate the correlation coefficient (see example).

 How does this outlier affect the correlation coefficient?



Excel Function NORM.INV(RAND(),0,1)

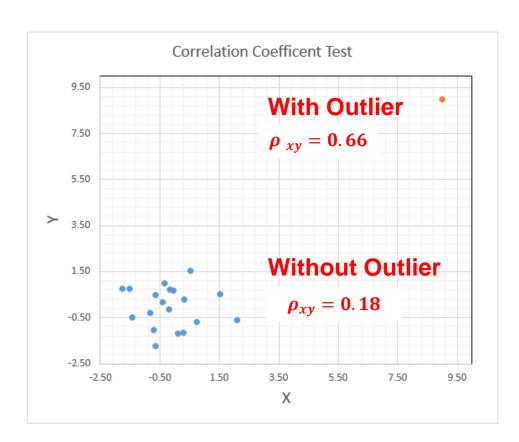
Exercise with Pearson's Correlation Coefficient



 Task 1: Generate a random data set of x and y variables and estimate their correlation coefficient (Hint: Rand() in Excel with N[0,1]).

 Task 2: Now add any desired outlier to the data and estimate the correlation coefficient (see example).

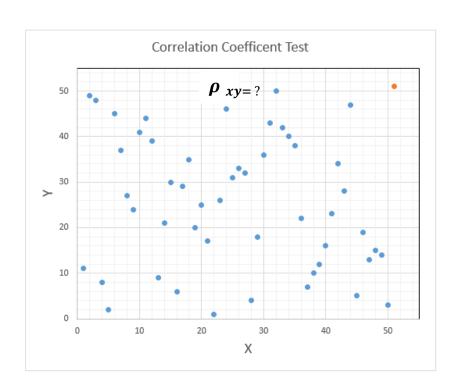
 How does this outlier affect the correlation coefficient?



Exercise with Pearson's Correlation Coefficient

 Task 3: Apply the rank transform to the dataset (Hint: 21-Rank.Avg() in Excel).

- How does this outlier now affect the correlation coefficient?
- This is a more robust form of the correlation coefficient called the rank correlation coefficient.



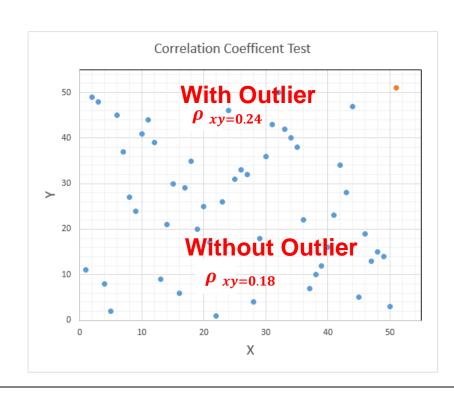
The Lines by of Texas at the

Exercise with Pearson's Correlation Coefficient

 Task 3: Applied the rank transform to the dataset

(Hint: 52-Rank.Avg() in Excel).

- How does this outlier now affect the correlation coefficient?
- This is a more robust form of the correlation coefficient called the rank correlation coefficient.

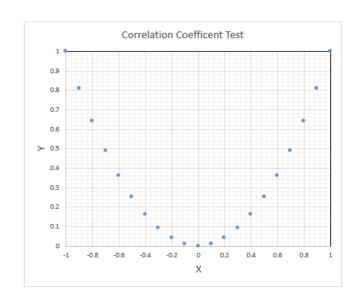


Excel Function =21-RANK.AVG(value,array)

Bivariate StatisticsMeasuring Linear Relationships with the Correlation Coefficient

Correlation / Covariance is a measure of linear relationship

What is the Correlation / Covariance of y
 x^2 over range of [-1, 1]?



Excel Function Correl(array1,array2)

Measuring Linear Relationships with the Correlation Coefficient

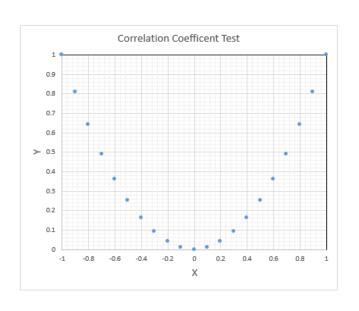
Correlation / Covariance is a measure of linear relationship

What is the Correlation / Covariance of y = x^2 over range of [-1, 1]?

Correlation Coefficient, $\rho_{xy} = 0.0!$



Correlation Coefficient, $\rho_{xy} = 0.96$, Rank Correlation Coefficient, $\rho_{RxRv} = 1.0$



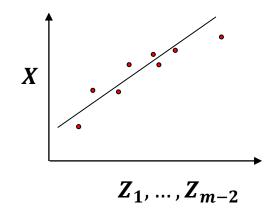
Excel Function Correl(array1,array2)

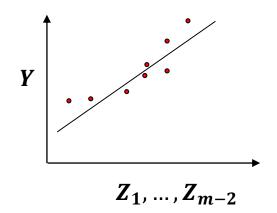
Bivariate StatisticsPartial Correlation



A method to calculate the correlation between X and Y after controlling for the influence of $Z_1, ..., Z_{m-2}$ other features on both X and Y.

- 1. perform linear, least-squares regression to predict X from Z_1, \ldots, Z_{m-2} . X is regressed on the predictors to calculate the estimate, X^*
- 2. perform linear, least-squares regression to predict Y from $Z_1, ..., Z_{m-2}$. Y is regressed on the predictors to calculate the estimate, Y^*



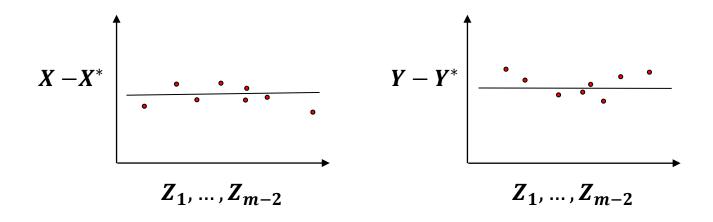


Bivariate StatisticsPartial Correlation



A method to calculate the correlation between X and Y after controlling for the influence of Z_1, \ldots, Z_{m-2} other features on both X and Y.

- 3. calculate the residuals in Step #1, $X X^*$, where $X^* = f(Z_1, ..., Z_{m-2})$, linear regression model
- 4. calculate the residuals in Step #1, $Y Y^*$, where $Y^* = f(Z_1, ..., Z_{m-2})$, linear regression model

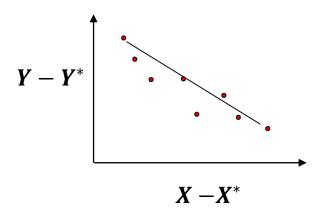


Bivariate StatisticsPartial Correlation



A method to calculate the correlation between X and Y after controlling for the influence of Z_1, \dots, Z_{m-2} other features on both X and Y.

5. calculate the correlation coefficient between the residuals from Steps #3 and #4, $\rho_{X-X^*,Y-Y^*}$



The partial correlation, provides a measure of the linear relationship between X and Y while controlling for the effect of Z_1, \ldots, Z_{m-2} other features on both, X and Y.

Partial Correlation Hands-on in Excel

Experiment with Partial Correlation:

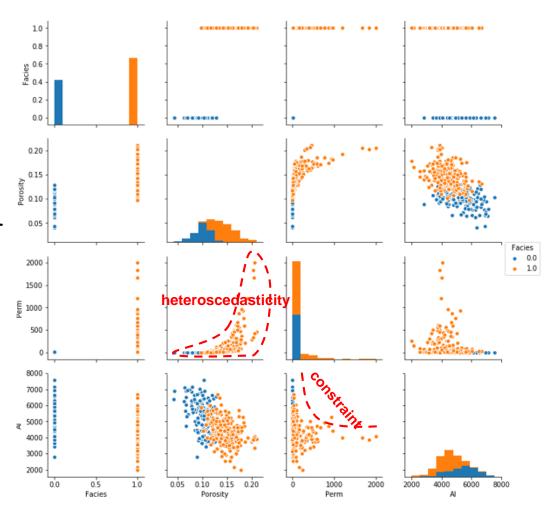


Things to try:

- 1. Increase the frequency over a region in the joint frequency distribution.
- 2. Add a TOC, Production outlier. TOC = 10, Production = 9999. What happened? Does Vsh inform porosity?

Bivariate Statistics Matrix Scatter Plots

- For more than two variables make matrix scatterplots
 - By hand in Excel or packages in R and Python.
 - Look for linear / nonlinear features
 - Look for homoscedasticity (constant conditional variance) and heteroscedasticity (conditional variance changes with value)
 - Look for constraints



Multivariate Modeling: Multivariate

Lecture outline . . .

Joints and Conditionals

Introduction

Fundamental Concepts

Probability

Data Prep / Analytics

Spatial Continuity / Prediction

Multivariate Modeling

Uncertainty Modeling

Machine Learning

Instructor: Michael Pyrcz, the University of Texas at Austin

Probability Definitions



Conditional, Marginal and Joint Probability

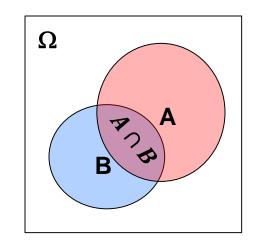
Probability of B given A occurred? P(B|A)

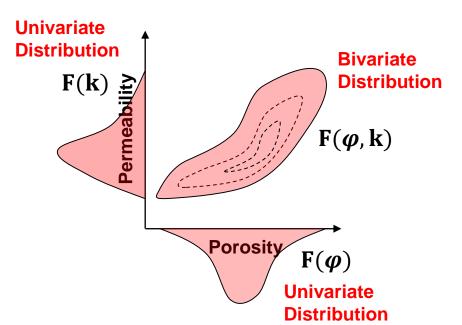
Joint Probability

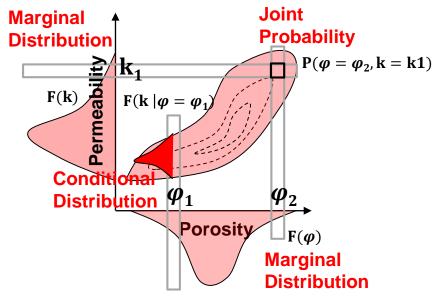
P(A O B) P(A and B)

$$P(B \mid A) = \frac{P(A \cap B)}{P(A)} = \frac{P(A \text{ and } B)}{P(A)}$$

Marginal Probability







Probability Definitions Conditional, Marginal and Joint Probability



Marginal Probability: Probability of an event, irrespective of any other event P(X), P(Y)

Conditional Probability: Probability of an event, given another event is already true.

$$P(X \ given \ Y), P(Y \ given \ X)$$

$$P(X \mid Y), P(Y \mid X)$$

Joint Probability: Probability of multiple events occurring together.

P(X and Y), P(Y and X)

 $P(X \cap Y), P(Y \cap X)$

P(X,Y), P(Y,X)

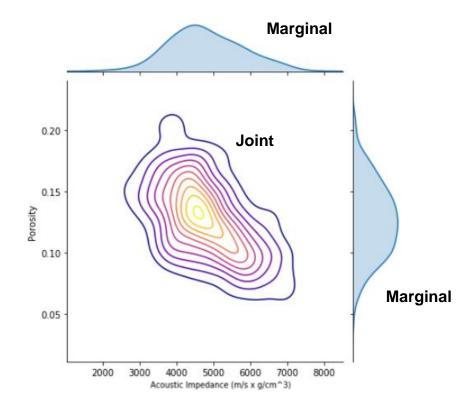


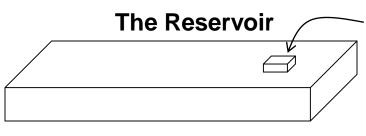
02c Geostatistics Course: Marginal, Conditional & Joint Probabilit

See YouTube Video on Marginals, Conditionals and

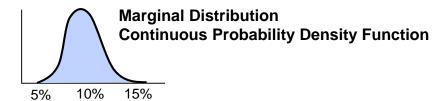
Joints! https://www.youtube.com/watch?v=bL2gPwMfYpc&index=5&t=0s&list=PLG19vXLQHvSB-

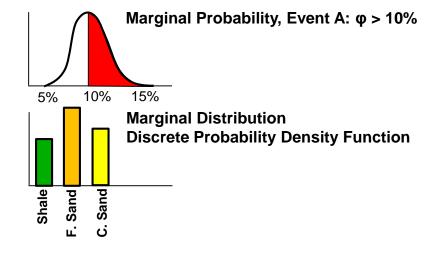
- Working directly with marginal, conditional and joint probability
 - If you have enough data, you can directly calculate all the required probabilities
 - Go beyond statistics like correlation coefficient

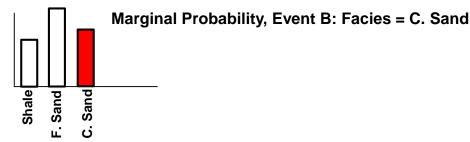




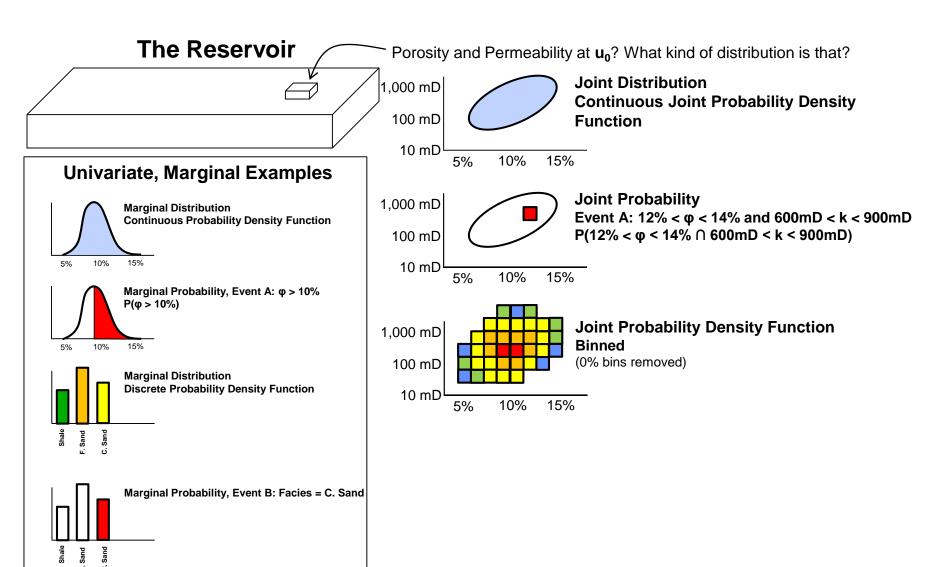
Porosity at $\mathbf{u_0}$? What kind of distribution is that?



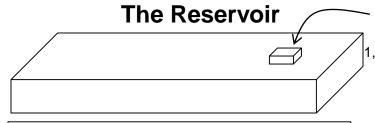




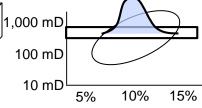




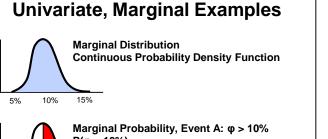


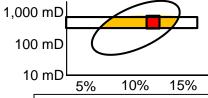


Permeability Given Porosity = φ_1 at u_0 ? What kind of distribution is that?

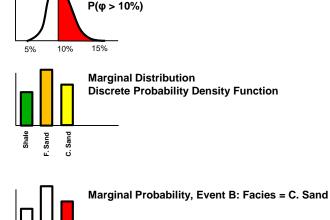


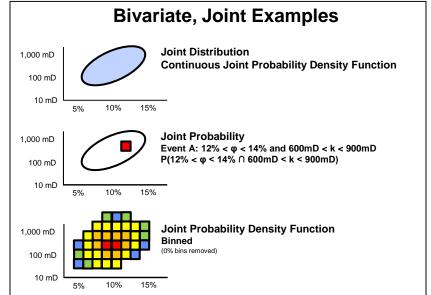
Conditional Distribution
Continuous Conditional Probability Density
Function





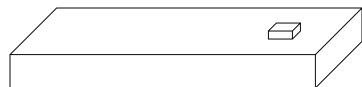
Conditional Probability
Event A: 12% < φ < 14% | 600mD < k < 900mD
P(12% < φ < 14% | 600mD < k < 900mD)



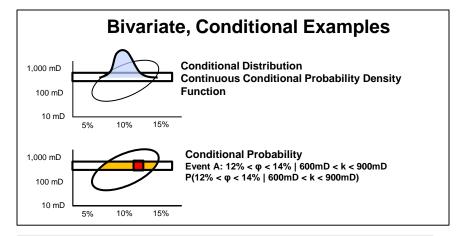


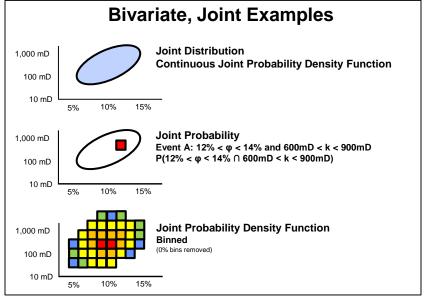


The Reservoir



Univariate, Marginal Examples Marginal Distribution Continuous Probability Distribution Function 15% 10% Marginal Probability, Event A: $\varphi > 10\%$ $P(\phi > 10\%)$ 10% 15% **Marginal Distribution Discrete Probability Distribution Function** Marginal Probability, Event B: Facies = C. Sand





and Joint Probability



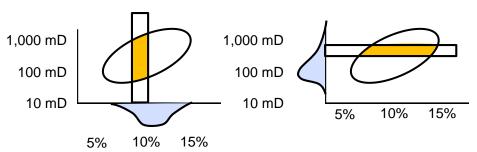


How to Calculate a Marginal Distribution from a Joint Distribution?

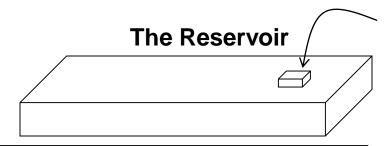


Definition of a Marginal Distribution

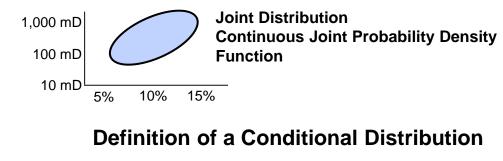
$$f_X(x) = \int_{-\infty}^{+\infty} f_{XY}(x, y) dy$$
 or $f_Y(y) = \int_{-\infty}^{+\infty} f_{XY}(x, y) dx$







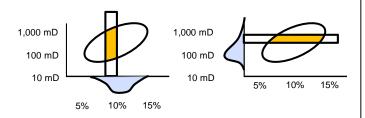
Calculate a Conditional Distribution from a Joint Distribution?



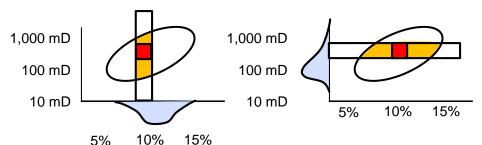
Definition of a Marginal Distribution

$$f_X(x) = \int_{-\infty}^{+\infty} f_{XY}(x, y) dy$$
 or $f_Y(y) = \int_{-\infty}^{+\infty} f_{XY}(x, y) dx$

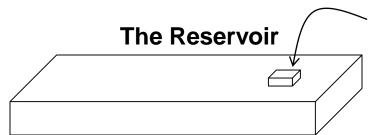
or
$$f_Y(y) = \int_{-\infty}^{+\infty} f_{XY}(x,y) dx$$



$$f_{Y|X}(y \mid x) = \frac{f_{XY}(x, y)}{f_X(x)}$$
 or $f_{X|Y}(x \mid y) = \frac{f_{XY}(x, y)}{f_Y(y)}$





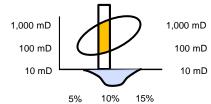


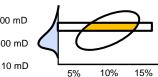
How to Calculate a Joint Distribution?

Definition of a Marginal Distribution

$$f_X(x) = \int_{-\infty}^{+\infty} f_{XY}(x, y) dy$$

$$f_X(x) = \int_{-\infty}^{+\infty} f_{XY}(x, y) dy$$
 or $f_Y(y) = \int_{-\infty}^{+\infty} f_{XY}(x, y) dx$





Definition of a Conditional Distribution

$$f_{Y|X}(y \mid x) = \frac{f_{XY}(x, y)}{f_X(x)}$$
 or $f_{X|Y}(x \mid y) = \frac{f_{XY}(x, y)}{f_Y(y)}$

1,000 mD

100 mD

100 mD

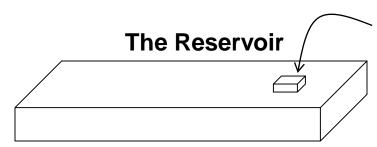
100 mD

5%

10%

15%



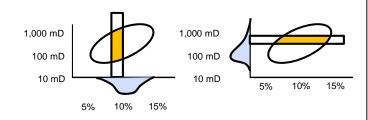


How to Calculate a Joint Distribution?

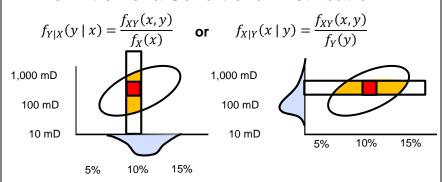
Definition of a Marginal Distribution

$$f_X(x) = \int_{-\infty}^{+\infty} f_{XY}(x, y) dy$$

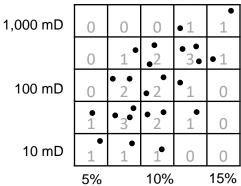
$$f_X(x) = \int_{-\infty}^{+\infty} f_{XY}(x, y) dy$$
 or $f_Y(y) = \int_{-\infty}^{+\infty} f_{XY}(x, y) dx$



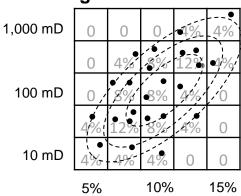
Definition of a Conditional Distribution



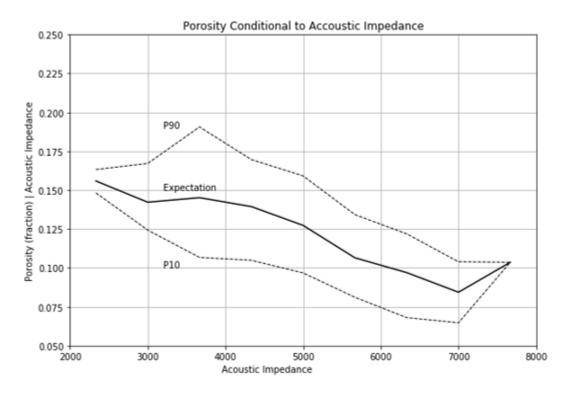
Non-parametric - Counting Samples in Bins



Fitting a Parametric Model



- Consider working with conditional statistics.
 - Powerful, flexible assessment of multivariate relationships, without linear assumption





Joint Distribution:

$$f_{XY}(x,y)$$

Marginal Distribution:

$$f_X(x) = \int_{-\infty}^{+\infty} f_{XY}(x, y) dy$$

Conditional Distribution:

$$f_{X|Y}(x \mid y) = \frac{f_{XY}(x, y)}{f_Y(y)}$$

Table of Frequencies

		400/	200/	E 00/	700/	000/
	2%	0	0	1	1	1
Porosity (%)	10%	0	0	2	3	2
	15% 20%	1	2	2	1	0
	20%	2	3	2	0	0
	25%	1	1	0	0	0

10% 30% 50% 70% 90% Fraction Shale (%)



Joint Distribution:

$$f_{XY}(x,y)$$

Marginal Distribution:

$$f_X(x) = \int_{-\infty}^{+\infty} f_{XY}(x, y) dy$$

Conditional Distribution:

$$f_{X|Y}(x \mid y) = \frac{f_{XY}(x, y)}{f_Y(y)}$$

Table of Joint Probabilities

25%	4%	4%	0	0	0
20%	8%	12%	8%	0	0
15%	4%	8%	8%	4%	0
10%	0	0	8%	12%	8%
2%	0	0	4%	4%	4%
	10% 15% 20%	8% 4% 0	%07 8% 12% 4% 8% 0 0	%07 8% 12% 8% 4% 8% 8% 0 0 8%	8% 12% 8% 0 4% 8% 8% 4% 0 0 8% 12%

10% 30% 50% 70% 90% Fraction Shale (%)



Given these joint probabilities calculate the: Table of Joint Probabilities

Marginal Distributions:

Vsh
 10%
 30%
 50%
 70%
 90%

$$f_{Vsh}(v_{sh})$$
 |
 |
 |
 |
 |
 |

 Porosity
 5%
 10%
 15%
 20%
 25%

 $f_{\varphi}(\varphi)$
 |
 |
 |
 |
 |

Porosity (%)	25 %	4%	4%	0	0	0
	20%	8%	12%	8%	0	0
	15%	4%	8%	8%	4%	0
	10%	0	0	8%	12%	8%
	2%	0	0	4%	4%	4%

10% 30% 50% 70% 90%

Conditional Distribution:

10% 30% 50% 70% 90%

 $f_{Vsh|\varphi}(v_{sh}|\varphi=15\%)=$

Fraction Shale (%)



Given these joint probabilities calculate the: Table of Joint Probabilities

Marginal Distributions:

Vsh 10% 30% 50% 70% 90%
$$f_{Vsh}(v_{sh})$$
 16% 24% 28% 20% 12%

Conditional Distribution:

(%)	
Porosity	

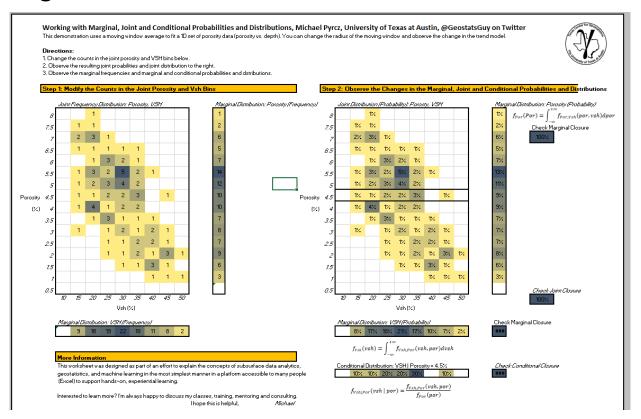
4%	4%	0	0	0
8% 12%		8%	0	0
4% 8%		8%	4%	0
0 0		8%	12%	8%
0	0	4%	4%	4%
	8% 4% 0	8% 12% 4% 8% 0 0	8% 12% 8% 4% 8% 8% 0 0 8%	8% 12% 8% 0 4% 8% 8% 4% 0 0 8% 12%

10% 30% 50% 70% 90% Fraction Shale (%)

$$f_{Vsh|\varphi}(v_{sh}|\varphi=15\%) = f_{Vsh,\varphi}(v_{sh},\varphi=15\%)/f_{\varphi}(\varphi=15\%)$$

Spatial Calculation in Hands-on in Excel

Experiment with Marginal, Joint and Conditionals:



Things to try:

- 1. Increase the frequency over a region in the joint frequency distribution.
- 2. Does Vsh inform porosity?

The file is Marginal_Joint_Conditional.xlsx at location https://git.io/fhA9X.

Multivariate Analysis Demo



GeostatsPy: Multivariate Analysis for Subsurface Data Analytics in Python

Michael Pyrcz, Associate Professor, University of Texas at Austin

Twitter | GitHub | Website | GoogleScholar | Book | YouTube | LinkedIn

PGE 383 Exercise: Multivariate Analysis for Subsurface Data Analytics in Python

Here's a simple workflow, demonstration of multivariate analysis for subsurface modeling workflows. This should help you get started with building subsurface models that integrate uncertainty in the sample statistics.

Bivariate Analysis

Understand and quantify the relationship between two variables

- · example: relationship between porosity and permeability
- · how can we use this relationship?

What would be the impact if we ignore this relationship and simply modeled porosity and permeability independently?

- · no relationship beyond constraints at data locations
- · independent away from data
- · nonphysical results, unrealistic uncertainty models

Bivariate Statistics

Pearson's Product-Moment Correlation Coefficient

- Provides a measure of the degree of linear relationship.
- . We refer to it as the 'correlation coefficient'

Let's review the sample variance of variable x. Of course, I'm truncating our notation as x is a set of samples a locations in our modeling space, $x(\mathbf{u}_{\alpha})$, $\forall \alpha = 0, 1, \dots, n-1$.

$$\sigma_x^2 = \frac{\sum_{i=1}^n (x_i - \bar{x})^2}{(n-1)}$$

We can expand the the squared term and replace on of them with y, another variable in addition to x.

$$C_{xy} = \frac{\sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y})}{(n-1)}$$

We now have a measure that represents the manner in which variables x and y co-vary or vary together. We can standardized the covariance by the product of the standard deviations of x and y to calculate the correlation coefficient.

$$\rho_{xy} = \frac{\sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y})}{(n-1)\sigma_x \sigma_x}, -1.0 \le \rho_{xy} \le 1.0$$

In summary we can state that the correlation coefficient is related to the covariance as:

$$\rho_{xy} = \frac{C_{xy}}{\sigma_x \sigma_y}$$

The Person's correlation coefficient is quite sensitive to outliers and depature from linear behavoir (in the bivariate sense). We have an alternative known as the Spearman's rank correlations coefficient.

Demo workflow for Multivariate Analysis

https://git.io/fh2DR

Multivariate Topics



- Other Topics that Could be Covered
 - Methods to remove correlation and model variables independently
 - Methods for dimensional reduction
 - Methods for clustering analysis

Topic	Application to Subsurface Modeling			
Multivariate Analysis	In the presence of multivariate relationships, must jointly model variables. Summarize with bivariate statistics, and visualize and use conditional statistics to go beyond linear measures.			
Limitations of Correlation	Correlation indicates degree of linear correlation and does not imply causation. Visualize and use rank correlation coefficient when needed and apply careful experiments (controlled) to establish causation.			
Use Conditional Statistics	Use conditional distributions to communicate the influence of variables on each other. Provides the value of knowing X to predict Y. Assess the influence of acoustic impedance on predicting porosity away from wells with conditional distributions.			

Multivariate Modeling: Multivariate

Lecture outline . . .

Feature Selection

Introduction

Fundamental Concepts

Probability

Data Prep / Analytics

Spatial Continuity / Prediction

Multivariate Modeling

Uncertainty Modeling

Machine Learning

Instructor: Michael Pyrcz, the University of Texas at Austin

Feature Ranking Motivation



Variable Ranking

- There are often many predictor features, input variables, available for us to work with for subsurface prediction.
- There are good reasons to be selective, throwing in every possible feature is not a good idea!
- In general, for the best prediction model, careful selection of the fewest features that provide the most amount of information is the best practice.

Feature Ranking Motivation



More Motivation to Work with Fewer Variables:

- more variables result in more complicated workflows that require more professional time and have increased opportunity for blunders
- higher dimensional feature sets are more difficult to visualize
- more complicated models may be more difficult to interrogate, interpret and QC
- inclusion of highly redundant and colinear variables increases model instability and decreases prediction accuracy in testing
- more variables generally increase the computational time required to train the model and the model may be less compact and portable
- the risk of overfit increases with the more variables, more complexity

What is Feature Ranking?



More Motivation to Work with Fewer Variables:

- Feature ranking is a set of metrics that assign relative importance or value to each feature with respect to information contained for inference and importance in predicting a response feature.
- There are a wide variety of possible methods to accomplish this.
- My recommendation is a wide-array approach with multiple metric, while understanding the assumptions and limitations of each metric.

Here's the general types of metrics that we will consider for feature ranking:

- 1. Visual Inspection of Data Distributions and Scatter Plots
- 2. Statistical Summaries
- 3. Model-based
- 4. Recursive Feature Elimination

What is Feature Ranking?



Expert Knowledge:

- Also, we should not neglect expert knowledge.
- If additional information is known about physical processes, causation, reliability and availability of features this should be integrated into assigning feature ranks.
- We should be learning as we perform our analysis, testing new hypotheses.



Metric #1: Visual Inspection

- In any multivariate work we should start with the univariate analysis, summary statistics of one variable at a time. The summary statistic ranking method is qualitative, we are asking:
 - are there data issues?
 - do we trust the features? do we trust the features all equally?
 - are there issues that need to be taken care of before we develop any multivariate workflows?



Summary statistics are a critical first step in data checking.

	count	mean	std	min	25%	50%	75%	max
Well	200.0	100.500000	57.879185	1.000000	50.750000	100.500000	150.250000	200.000000
Por	200.0	14.991150	2.971176	6.550000	12.912500	15.070000	17.402500	23.550000
Perm	200.0	4.330750	1.731014	1.130000	3.122500	4.035000	5.287500	9.870000
AI	200.0	2.968850	0.566885	1.280000	2.547500	2.955000	3.345000	4.630000
Brittle	200.0	48.161950	14.129455	10.940000	37.755000	49.510000	58.262500	84.330000
TOC	200.0	0.991950	0.478264	0.000000	0.617500	1.030000	1.350000	2.180000
VR	200.0	1.964300	0.300827	0.930000	1.770000	1.960000	2.142500	2.870000
Prod	200.0	3864.407081	1553.277558	839.822063	2686.227611	3604.303507	4752.637556	8590.384044
const	200.0	1.000000	0.000000	1.000000	1.000000	1.000000	1.000000	1.000000

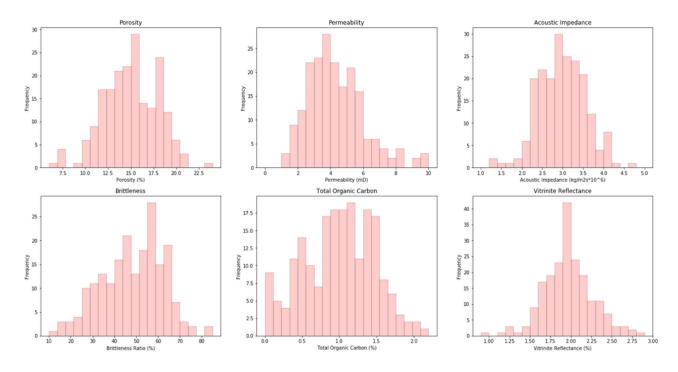
- the number of valid (non-null) values for each feature
- general behaviors such as central tendency, mean, and dispersion, variance.
- issues with negative values, extreme values, and values that are outside the range of plausible values for each property.



Metric #2: Univariate Distributions

- As with summary statistics, this ranking method is a qualitative check for issues with the data and to assess our confidence with each feature.
- It is better to not include a feature with low confidence of quality as it may be misleading (while adding to model complexity as discussed previously).
- Assess our ability to use methods that have distribution assumptions





The univariate distributions look good:

- there are no obvious outliers
- the permeability is positively skewed as often observed
- the corrected TOC has a small zero truncation spike, but it's reasonable
- some departure from Gaussian form, could transform



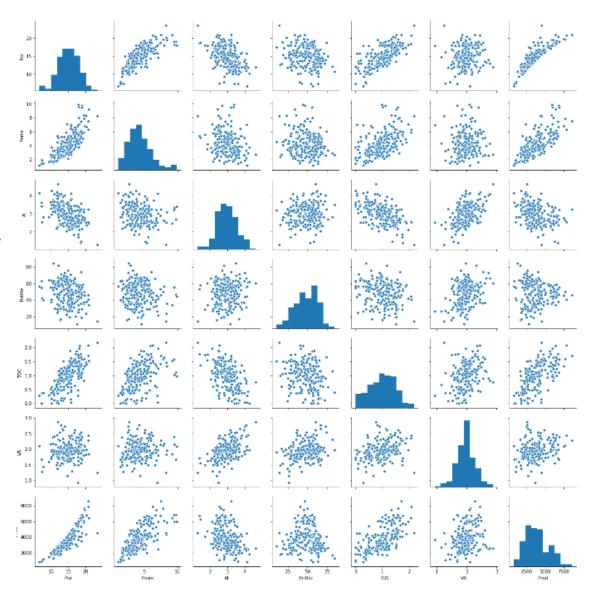
Metric #3: Bivariate

- matrix scatter plots are a very efficient method to observe the bivariate relationships between the variables.
- this is another opportunity through data visualization to identify data issues, outliers
- we can assess if we have collinearity, specifically the simpler form between two features at a time
- Bivariate Gaussian is assumed for methods such as correlation and partial correlation



How could we use this plot for variable ranking?

- variables that are closely related to each other.
- linear vs. non-linear relationships
- constraint relationships and heteroscedasticity between variables.





Metric #3: Bivariate

- bivariate visualization and analysis is not sufficient to understand all the multivariate relationships in the data
- multicollinearity includes strong linear relationships between 2 or more features.
- higher order nonlinear features, outliers and coverage?
- these may be hard to see with only bivariate plots.



Ranking Method #4 - Pairwise Covariance

- Pairwise covariance provides a measure of the strength of the linear relationship between each predictor feature and the response feature.
- We now specify our goal of this study is to predict production, our response variable, from the other available predictor features.
- We are thinking predictively now, not inferentially, we want to estimate the function, \hat{f} to accomplish this

Covariance:

- measures the strength of the linear relationship between features
- sensitive to the dispersion / variance of both the predictor and response



Ranking Method #4 - Pairwise Covariance

- Sensitive to feature variance
- Feature variance is somewhat arbitrary.
 - For example, what is the variance of porosity in fraction vs.
 percentage or permeability in Darcy vs. milliDarcy. We can show
 that if we apply a constant multiplier, cc, to a variable, XX, that the
 variance will change according to this relationship (the proof is
 based on expectation formulation of variance):

$$\sigma_{cX}^2 = c^2 \sigma_X^2$$

- By moving from percentage to fraction we decrease the variance of porosity by a factor of 10,000!
- The variance of each variable is potentially arbitrary, with the exception when all the features are in the same units.



Ranking Method #5 - Pairwise Correlation Coefficient

- Pairwise correlation coefficient provides a measure of the strength of the linear relationship between each predictor feature and the response feature.
- The correlation coefficient:
 - measures the linear relationship
 - removes the sensitivity to the dispersion / variance of both the predictor and response features, by normalizing by the product of the standard deviation of each feature



Ranking Method #6 – Rank Correlation Coefficient

- The rank correlation coefficient applies the rank transform to the data prior to calculating the correlation coefficient. To calculate the rank transform simply replace the data values with the ranks, where n is the maximum value and 1 is the minimum value.
- The rank correlation:
 - measures the monotonic relationship, relaxes the linear assumption
 - removes the sensitivity to the dispersion / variance of both the predictor and response, by normalizing by the product of the standard deviation of each.



Ranking Method #7 – Partial Correlation Coefficient

This is a linear correlation coefficient that controls for the effects all the remaining variables

- $\rho_{XY,Z}$ and is the partial correlation between X and Y after controlling for Z.
- 1. perform linear, least-squares regression to predict X from $Z_{1,\dots,m-2}$.
- 2. calculate the residuals in Step #1, $X X^*$
- 3. perform linear, least-squares regression to predict Y from $Z_{1,\dots,m-2}$.
- 4. calculate the residuals in Step #1, $Y Y^*$
- 5. calculate the correlation coefficient, $\rho_{XY,Z} = \rho_{X-X^*,Y-Y^*}$



Ranking Method #7 – Partial Correlation Coefficient

The partial correlation, provides a measure of the linear relationship between X and Y while controlling for the effect of Z other features on both, X and Y

To use this method we must assume:

- two variables to compare, X and Y
- other variables to control, $Z_{1,\dots,m-2}$.
- linear relationships between all variables
- no significant outliers
- approximately bivariate normality between the variables

We are in pretty good shape, but we have some departures from bivariate normality.

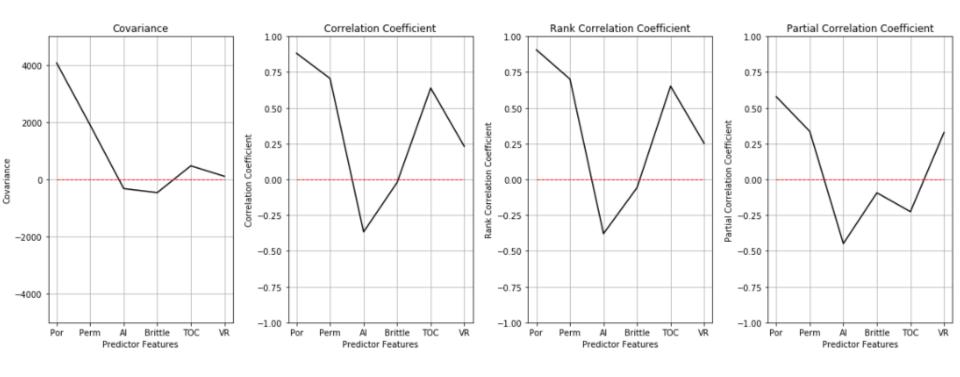
We apply a Gaussian transform in the demonstration



Ranking Methods #4 - #7 - Results

Are we converging on porosity, permeability and vitrinite reflectance as the most important variables with respect to linear relationships with the production?

What about brittleness?





Ranking Method # 9 – Model-based Ranking – B coefficients

 We could also consider B coefficients from linear regression.

$$Y^* = \sum_{i=1}^m B_i X_i + c$$

- These are the linear regression coefficients without standardization of the variables.
- Sensitive to feature variance.
- We are capturing interactions between variables.



Ranking Method # 9 – Model-based Ranking – B (beta) coefficients

We could also consider B coefficients from linear regression

$$Y^{S*} = \sum_{i=1}^{m} B_i X_i^S + c$$

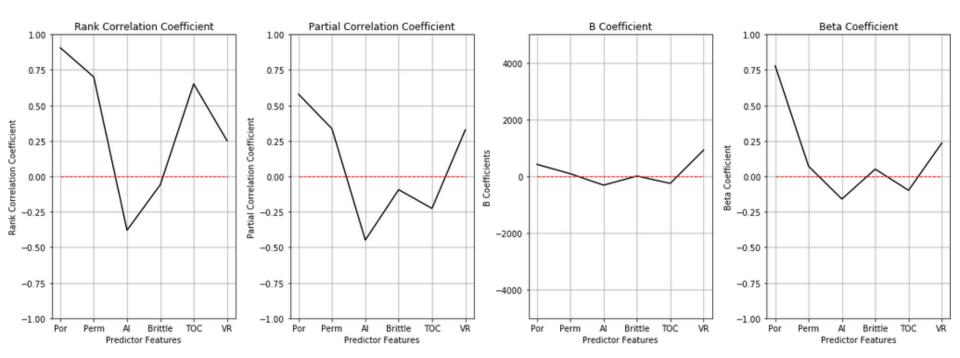
- These are the linear regression coefficients with standardization of the variables, X_i^s and Y^{s*} (variance = 1)
- Not sensitive to variance of the features
- We are capturing interactions between variables.



Ranking Methods #4 - #9 - Results

Now what do we see?

- Beta demotes permeability!
- Porosity, acoustic impedance and vitrinite reflectance retain high metrics





Ranking Methods #11– Recursive Feature Elimination

Recursive Feature Elimination (RFE) method works by recursively removing features and building a model with the remaining features.

- model accuracy is applied to identify which attributes (and combination of attributes) contribute the most to predicting the target attribute
- any model could be used!
- in this example the prediction model based on multilinear regression and indicate that we want to find the best feature based on recursive feature elimination.
- the method assigns rank 1, ..., m for all features.



Ranking Methods #11– Recursive Feature Elimination

The recursive feature elimination method with a linear regression model provides these ranks:

- 1. Total Organic Carbon
- 2. Vitrinite Reflectance
- 3. Acoustic Impedance
- 4. Porosity
- 5. Permeability
- 6. Brittleness

A couple of the features moved from our previous assessment, but we are close. The advantages with the recursive elimination method:

- the actual model can be used in assessing feature ranks
- the ranking is based on accuracy of the estimate



Ranking Methods #11– Recursive Feature Elimination

The recursive feature elimination method with a linear regression model provides these ranks, but this method is sensitive to:

- choice of model
- training dataset

This method may be applied with cross validation (k fold iteration of training and testing datasets)

 optimize variable selection for prediction with testing data after training with training data

Feature Ranking Demonstration in Python

Demonstration of the wide array approach with a documented workflow.

GeostatsPy: Multivariate Analysis for Subsurface Data Analytics in Python

Michael Pyrcz, Associate Professor, University of Texas at Austin

Twitter | GitHub | Website | GoogleScholar | Book | YouTube | LinkedIn

Subsurface Machine Learning: Feature Ranking for Subsurface Data Analytics

Here's a demonstration of feature ranking for subsurface modeling in Python. This is part of my Subsurface Machine Learning Course at the Cockrell School of Engineering at the University of Texas at Austin.

Variable Ranking

There are often many predictor features, input variables, available for us to work with for subsurface prediction. There are good reasons to be selective, throwing in every possible feature is not a good idea! In general, for the best prediction model, careful selection of the fewest features that provide the most amount of information is the best practice.

Here's why:

- more variables result in more complicated workflows that require more professional time and have increased opportunity for blunders
- higher dimensional feature sets are more difficult to visualize
- more complicated models may be more difficult to interrogate, interpret and QC
- inclusion of highly redundant and colinear variables increases model instability and decreases prediction accuracy in testing
- more variables generally increase the computational time required to train the model and the model may be less compact and portable
- · the risk of overfit increases with the more variables, more complexity

What is Feature Ranking?

Feature ranking is a set of metrics that assign relative importance or value to each feature with respect to information contained for inference and importance in predicting a response feature. There are a wide variety of possible methods to accomplish this. My recommendation is a 'wide-array' approach with multiple metric, while understanding the assumptions and limitations of each metric.

Here's the general types of metrics that we will consider for feature ranking.

- Visual Inspection of Data Distributions and Scatter Plots
 Statistical Summarion

Workflow at

https://github.com/GeostatsGuy/Pyth onNumericalDemos/blob/master/Geos tatsPy_variable_ranking.ipynb

Multivariate Modeling: Multivariate

Lecture outline . . .

Multivariate Estimation

Introduction

Fundamental Concepts

Probability

Data Prep / Analytics

Spatial Continuity / Prediction

Multivariate Modeling

Uncertainty Modeling

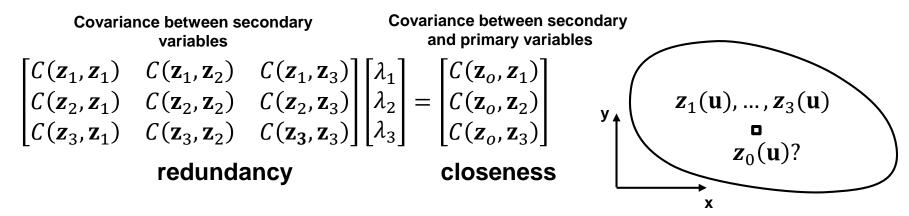
Machine Learning

Instructor: Michael Pyrcz, the University of Texas at Austin

Multivariate Kriging



- Simple kriging may be applied to make estimates given a set of collocated secondary variables at the location to estimate the primary variable.
- This is not spatial estimation, but multivariate estimation!



- Given the assumption of Gaussian distributed variables we have a complete model of uncertainty for the primary variable at location u!
- We can back transform for uncertainty in the original variable units.

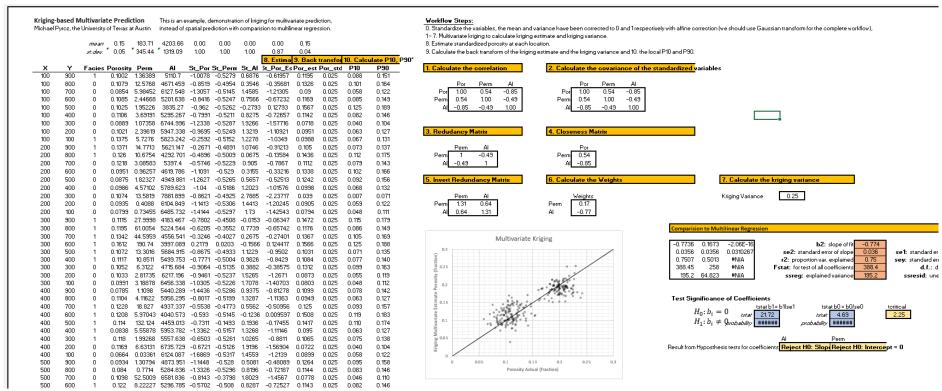
Multivariate Kriging Hands-on



Here's an opportunity for experiential learning with Simple Kriging for multivariate estimation and uncertainty.

Things to try:

Observe the multivariate weights, estimator and variance. Walk through the steps.



File Name: Kriging_Multivariate_Estimation_Demo.xlsx

File is at: https://git.io/fhALF

Topic	Application to Subsurface Modeling
Curse of Dimensionality	Reduce problem to lowest dimension possible.
	Feature ranking determined that porosity may be predicted from acoustic impedance and rock type alone.
Feature Selection	Apply wide array methods to explore the importance of each predictor feature with respect to the response feature.
	Partial correlation reveals that rock type provides little additional information to acoustic impedance.
	Multivariate kriging combines secondary information sources while accounting for closeness and redundancy.
Multivariate Kriging	Given secondary data the likelihood distribution for local porosity is mean of 15% and standard deviation of 2.5% with a Gaussian distribution.

Multivariate Modeling: Multivariate

Lecture outline . . .

- Multivariate Analysis
- Joints and Conditionals
- Feature Selection
- Multivariate Estimation

Introduction

Fundamental Concepts

Probability

Data Prep / Analytics

Spatial Continuity / Prediction

Multivariate Modeling

Uncertainty Modeling

Machine Learning

Instructor: Michael Pyrcz, the University of Texas at Austin