Subsurface Data Analytics and Machine Learning

Analytics and Machine Learning

Lecture outline . . .

- **General Comments**
- **Data Analytics**
- **Machine / Statistical Learning**
- **Prediction and Inference**

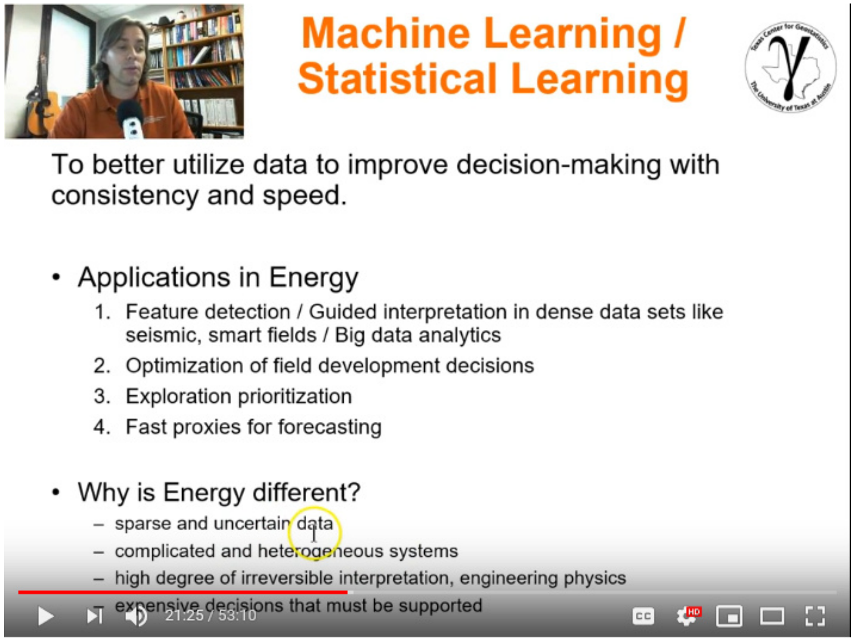
Instructor: Michael Pyrcz, the University of Texas at Austin

Subsurface Data Analytics and Machine Learning

Analytics and Machine Learning

Other Resources:

- **Recorded Lecture Statistical / Machine Learning**



Machine Learning / Statistical Learning

To better utilize data to improve decision-making with consistency and speed.

- Applications in Energy
  1. Feature detection / Guided interpretation in dense data sets like seismic, smart fields / Big data analytics
  2. Optimization of field development decisions
  3. Exploration prioritization
  4. Fast proxies for forecasting
- Why is Energy different?
  - sparse and uncertain data
  - complicated and heterogeneous systems
  - high degree of irreversible interpretation, engineering physics
  - expensive decisions that must be supported

Instructor: Michael Pyrcz, the University of Texas at Austin

Goals of This Lecture

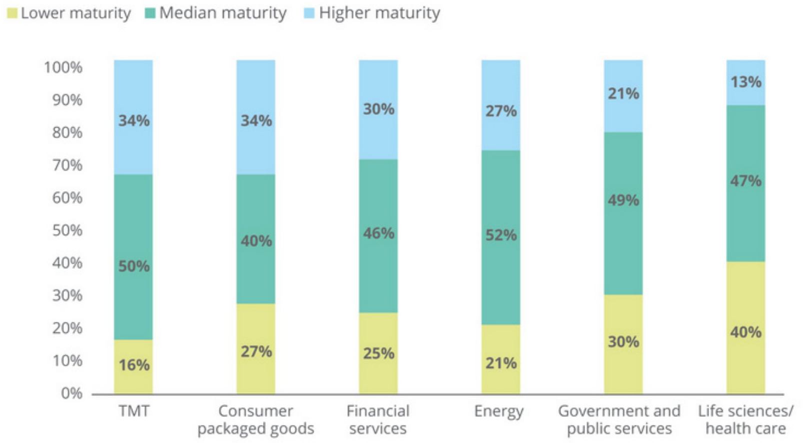
- Motivation
- My biases
- Definition of terms and introduce concepts
- Then we will dive into data analytics, followed by machine learning.

Digital Transformations

- We are not alone, digital transformations are underway in all sectors of our economy.
- Every energy company that I visit is working on this right now.

FIGURE 14

TMT companies had the greatest percentage of median- and higher-maturity organizations



Note: Percentages may not total 100% due to rounding.
Source: Deloitte Digital Transformation Executive Survey 2018.

Deloitte Insights | deloitte.com/insights

Digital transformation study by Deloitte, 2019.

https://www2.deloitte.com/insights/us/en/focus/digital-maturity/digital-maturity-pivot-model.html

Digital Transformations

My Biases:

- There are opportunities to do more with our data
- There are opportunities to teach data analytics and statistical / machine learning methods to engineers and geoscientists to improve capability
- Geoscience and engineering knowledge and expertise remains core to our business

Digital transformation PricewaterhouseCoopers (PwC) panel April, 9th, 2019.

Subsurface Data Analytics and Machine Learning

Data Analytics and Machine Learning

Lecture outline . . .

- **Data Analytics**

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Big Data

Big Data: you have big data if your data has a combination of these:

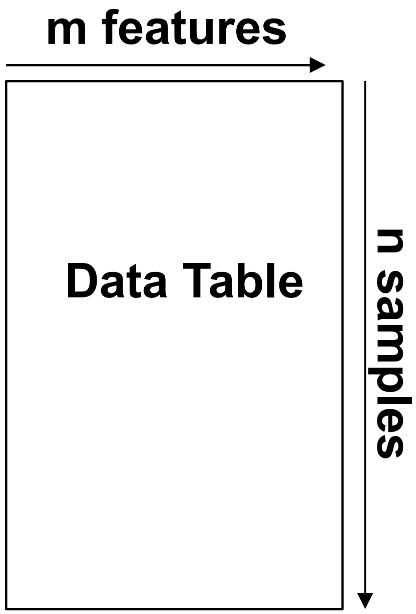
Volume: large number of data samples, large memory requirements and difficult to visualize

Velocity: data is gathered at a high rate, continuously relative to decision making cycles

Variety: data form various sources, with various types and scales

Variability: data acquisition changes during the project

Veracity: data has various levels of accuracy



m features

Data Table

n samples

“Energy has been big data before tech learned about big data.”
– Michael Pyrcz

Big Data Analytics – methods to explore and detect patterns, trends and other useful information from big data to improve decision making.

Big Data Analytics

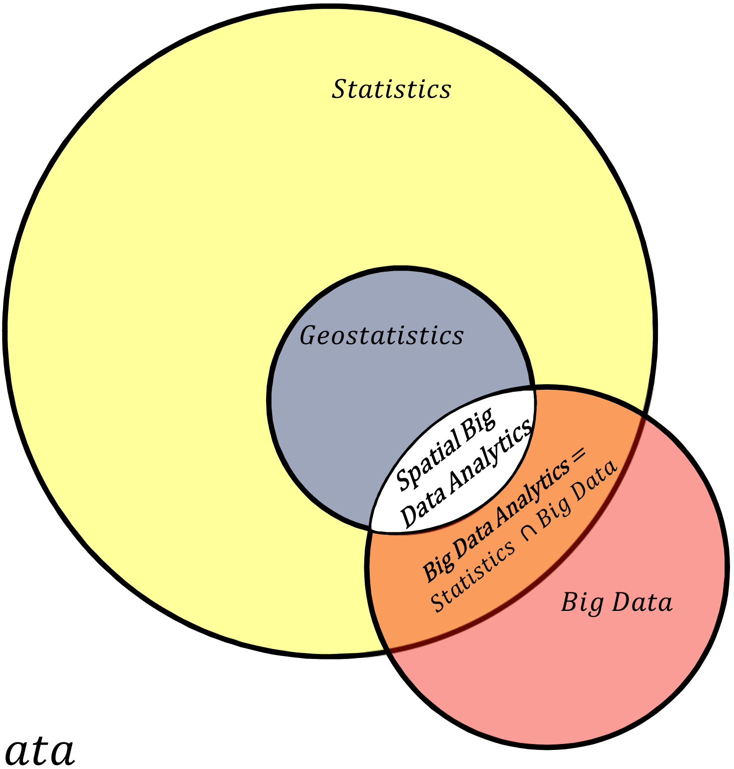
Statistics is collecting, organizing, and interpreting data, as well as drawing conclusions and making decisions.

Geostatistics is a branch of applied statistics: (1) the spatial (geological) context, (2) the spatial relationships, (3) volumetric support, and (4) uncertainty.

Big Data Analytics is the process of examining large and varied data sets (big data) to discover patterns and make decisions.

$$Spatial\ Big\ Data\ Analytics = Geostatistics\ \cap Big\ Data$$

Big data analytics is expert use of (geo)statistics on big data.


Statistics
Geostatistics
Spatial Big Data Analytics
Big Data Analytics = Statistics ∩ Big Data
Big Data

Proposed Venn diagram for spatial big data analytics.

Subsurface Data Analytics and Machine Learning

Analytics and Machine Learning

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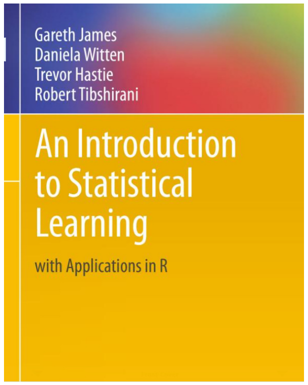
Machine Learning / Statistical Learning

- Excellent Reading on this Topic: An Introduction to Statistical Learning with Applications in R, 2013, James et al., Springer. (http://www-bcf.usc.edu/~gareth/ISL/ISLR%20First%20Printing.pdf)



Gareth James
Daniela Witten
Trevor Hastie
Robert Tibshirani

An Introduction to Statistical Learning

with Applications in R

- **Statistical Learning**
  - vast set of tools for learning from data
  - based on initial assumptions and hypothesis

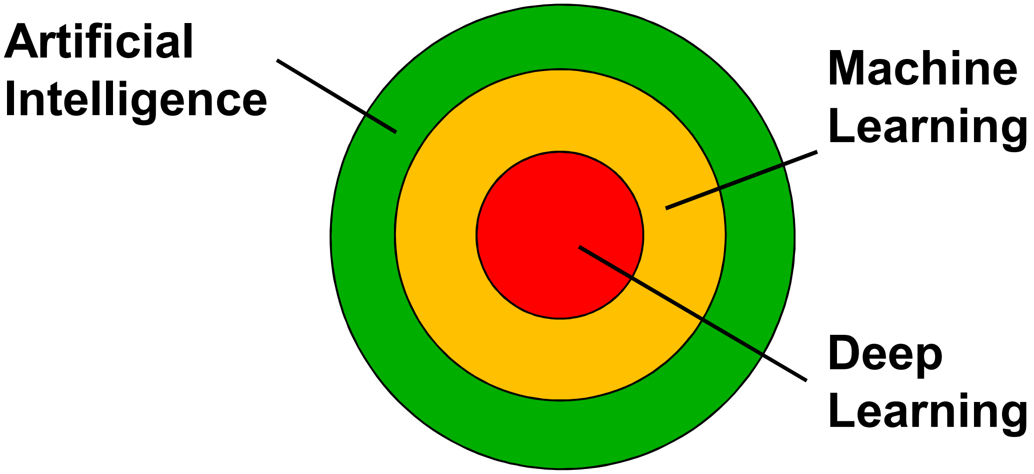
- **Machine Learning vs. Statistical Learning**
  - vast set of tools for learning patterns
  - very little if any prior assumptions

- **Supervised Learning**
  - building a predictive model for estimating an output given one or more inputs

- **Unsupervised Learning**
  - all inputs, no output
  - learn from the structures of the data alone

Note: Some consider statistical learning and machine learning to be the same
I'll use them interchangeably

Machine Learning / Statistical Learning



Artificial Intelligence

Machine Learning

Deep Learning

Artificial Intelligence: the theory and development of computer systems able to perform tasks that normally require human intelligence, such as visual perception, speech recognition, decision-making, and translation between languages (Google Dictionary)

Machine Learning: is an application of artificial intelligence (AI) that provides systems the ability to automatically learn and improve from experience without being explicitly programmed (Google Dictionary). Access data and learn for themselves.

Deep Learning: subset of machine learning with complicated neural nets

Machine Learning / Statistical Learning

Machine Learning:

toolkit

training
with data

“is the study of algorithms and mathematical models that computer systems use to progressively improve their performance on a specific task. Machine learning algorithms build a mathematical model of sample data, known as "training data", in order to make predictions or decisions without being explicitly programmed to perform the task.”

learning

general

“where it is infeasible to develop an algorithm of specific instructions for performing the task.”

not a panacea

Machine Learning - Wikipedia

Machine Learning / Statistical Learning

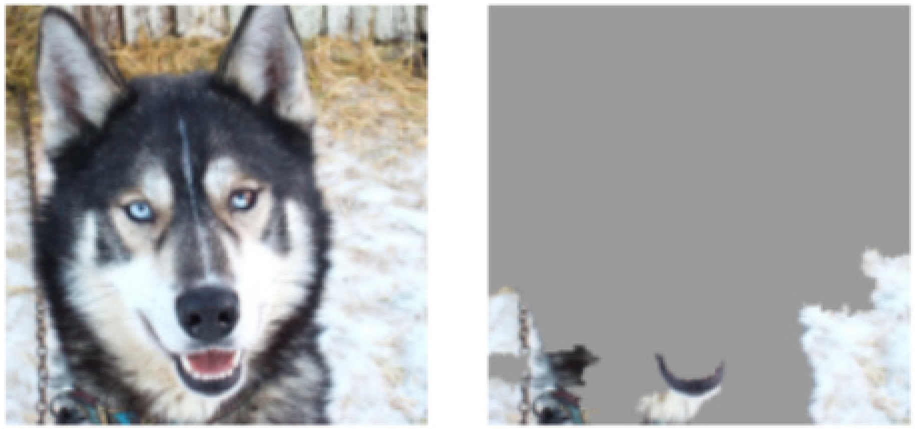
Concerns:

Biased training data

Rideiro et al. (2016) trained a logistic regression classifier with 20 wolves and dogs images to detect the difference between wolves and dogs.

The problem is:

- interpretability may be low
- application may become routine and trusted
- the machine is trusted, becomes an authority



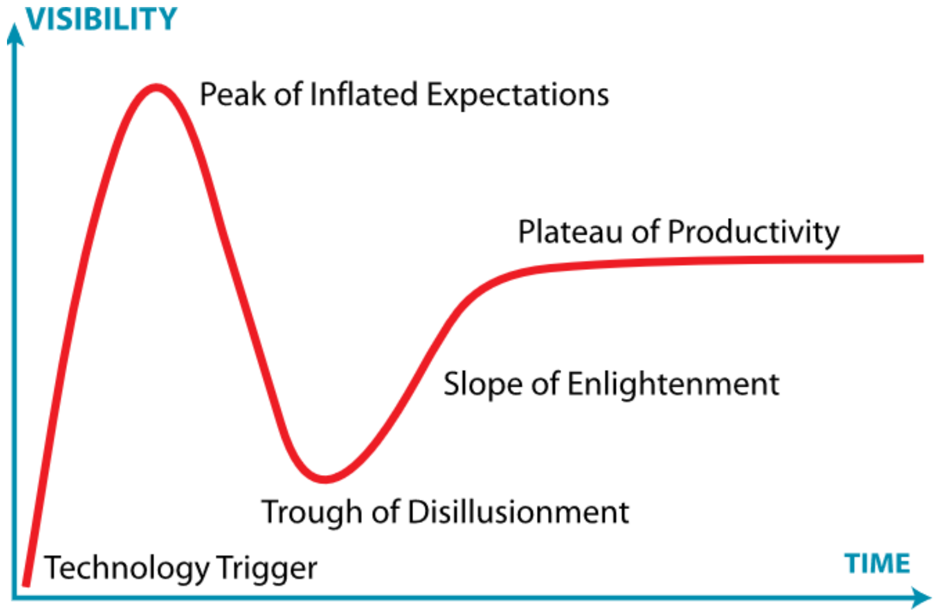
(a) Husky classified as wolf (b) Explanation

Figure 11: Raw data and explanation of a bad model's prediction in the "Husky vs Wolf" task.

Image and example from Ribeiro et al., (2016)
https://arxiv.org/pdf/1602.04938.pdf

Machine Learning / Statistical Learning

- Hype Cycle – from information technology firm, Gartner.



Where are we currently for data analytics and machine learning?

Image from https://en.wikipedia.org/wiki/Hype_cycle.

Machine Learning / Statistical Learning

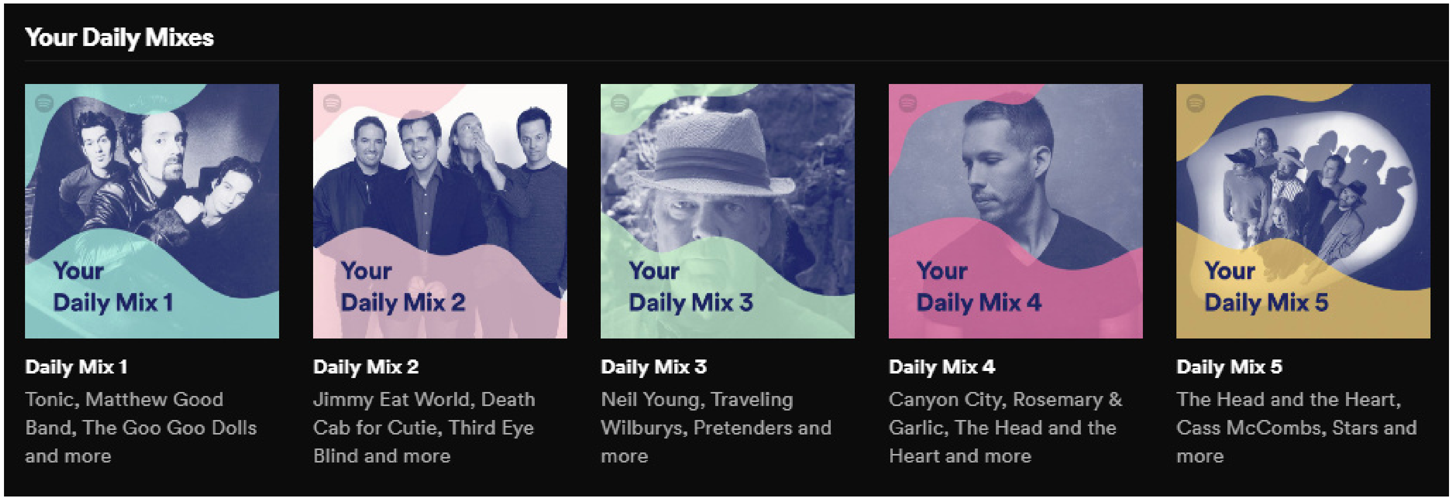
Applications Around You / Societal Impacts

1. Driving directions that crowd source and update improve traffic flow
2. Air traffic routing
3. Spam filters
4. Plagiarism checkers
5. Translation / computer reading
6. Credit card fraud detection
7. Face recognition (Facebook, Snapchat etc.)
8. Recommendations (Amazon, Netflix, YouTube)
9. Smart personal assistants

Machine Learning / Statistical Learning

But Energy is Very Different

- sparse and uncertain data
- complicated and heterogeneous, open earth systems
- high degree of **necessary geoscience and engineering interpretation and physics**
- **Expensive, high value decisions** that must be supported



Your Daily Mixes

Daily Mix 1
Tonic, Matthew Good Band, The Goo Goo Dolls and more

Daily Mix 2
Jimmy Eat World, Death Cab for Cutie, Third Eye Blind and more

Daily Mix 3
Neil Young, Traveling Wilburys, Pretenders and more

Daily Mix 4
Canyon City, Rosemary & Garlic, The Head and the Heart and more

Daily Mix 5
The Head and the Heart, Cass McCombs, Stars and more

Spotify recommendation engine, recommender system

Machine Learning / Statistical Learning

My recommendations for Machine Learning in Energy:

Support Subsurface Development when:

- volume of data is too large to queried by hand
- the system is high dimensional and cannot be explained with geoscience and engineering
- the task is routine, highly repetitive and low value

With systems that:

- Streamline and automate
- Support expert and system interaction
- Interrogatable with excellent visualization and diagnostics

Machine Learning / Statistical Learning

Example Machine Learning Applications in Energy

1. Feature detection / guided interpretation in dense data sets like seismic and smart fields
2. Expert systems to detect anomalous operating conditions for safe drilling
3. Optimization of field development decisions with the integration of all relevant geoscience and engineering interpretations and physics
4. Model feedback with fast proxies for geologic and engineering processes to provide guidance for subsurface interpretation and modeling.

“Significance, consistency, efficiency for more impact.”

Machine Learning / Statistical Learning

Data, Metadata and Databases

- 80% of any subsurface study is data preparation and interpretation
- We continue to face a challenge with data:
  - Data curation
  - Large volume
  - Large volumes of metadata
  - Variety of data, scale, collection, interpretation
  - Transmission, controls and security

- Databases are prerequisite to all data analytics and machine learning.

MetaData Definition

‘a set of data that describes and gives information about other data’ - Google dictionary

‘computing information that is held as a description of stored data’ – dictionary.com

- data collection, calibration, uncertainty, transformations, standardization, interpretation, correction, debiasing
- we have a massive amount of metadata

Skilled Use

Just like spatial statistics / geostatistics, statistical learning is a set of tools to add to your tool box as geoscientist or engineer

- Each is very dangerous to use as a black box. You will need to understand what’s under the hood
  - methods, workflows, assumptions and limitations.
  - scope and trade offs between alternative methods

Skilled Use

Imagine you are a carpenter (from Pyrcz and Deutsch, 2014).

- You would have a tool box
- You would know each tool perfectly well
- Understand performance over a variety of applications
- You would understand the range of applications, weaknesses, strengths, limits.
- Choice between tools would be based on expert judgement of circumstances and goals of a project
- You would choose specific tools to have ready for use and other for more rare circumstances
- Too few tools and a box overwhelmed with obscure tools are both issues.

Skilled Use

Hadley Wickham, Chief Scientist at RStudio, known for development of open-source statistical packages for R to make statistics accessible and fun (http://hadley.nz/).

Read Hadley Wickham's, **Teaching Safe-Stats, Not Statistical Abstinence** (https://nhorton.people.amherst.edu/mererenovation/17_Wickham.PDF)

- **Teaching:** We need to rethink statistics curriculum – we risk becoming irrelevant!
- **Practice:** Stats tends to be taught as avoid, unless you are an "statistician" or with one
    - Otherwise you will cause great harm
    - But there are not enough professional statisticians
    - Rather than stigmatize amateur, new tools should be safer to use
- **Tools**: New tools should be easy and fun to use to encourage use
    - Flexible grammars, minimal set of independent components to build workflows

Hadley Wickham photograph from https://en.wikipedia.org/wiki/Hadley_Wickham

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Analytics and Machine Learning

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The Model

Predictors, Independent Variables, Features

- input variables
- for a model $Y = f(X_1, \ldots, X_m) + \epsilon$, these are the $X_1, \ldots, X_m$
- note ϵ is a random error term

Response, Dependent Variables

- output variable
- for a model $Y = f(X_1, \ldots, X_m)$, this is Y

Statistical / Machine Learning is All About

- Estimating f for two purposes
  1. Prediction
  2. Inference

Inference

There is value in understanding the relationships between predictor features

- for $Y = f(X_1, \dots, X_m) + \epsilon$ we can understand the influence / interactions of each X_α on each other.

What is the relationship between each predictor feature?

- sense of the relationship (positive or negative)?
- shape of relationship (sweet spot)?
- relationships may depend on values of other predictors!

‘Inference is learning about the system.’

Prediction

Estimating, $\hat{f}$, for the purpose of predicting $\hat{Y}$

- We are focused on getting the most accurate estimates, $\hat{Y}$
- We may not even understand what is happening between the X's!
- We are concerned about the relationships between X and Y

'Prediction is modeling the system to make estimates, forecasts.'

Estimating f

Parametric Methods

- make an assumption about the functional form, shape
- we gain simplicity and advantage of only a few parameters
- for example, here is a linear model

$$Y = f(X) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_m X_m$$

- there is a risk that $\hat{f}$ is quite different than f, then we get a poor model!

Estimating f

Nonparametric Methods

– make no assumption about the functional form, shape

– more flexibility to fit a variety of shapes for f

– less risk that $\hat{f}$ is a poor fit for f

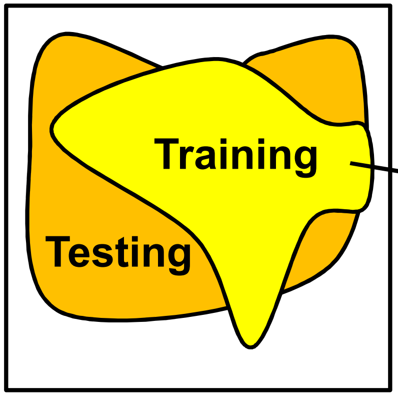
– typically need a lot more data for an accurate estimate of f

'Nonparametric is actually parametric rich!'

Training and Testing

The Training and Testing Workflow

Separate The Data



Train the Model

Train the Model Parameters Maximize Accuracy with Training Data

Tune the Model

Test the Model Tune the Hyperparameters to Optimize the Complexity

We avoid the overfit problem.

Model Parameters Definition

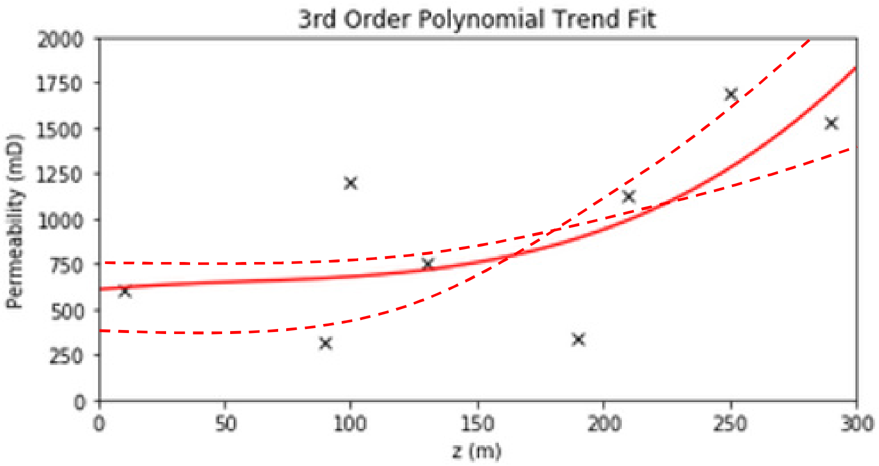
Model Parameters

Derived during training phase to fit the model to the training data

Parameters

$$k = b_3 z^3 + b_2 z^2 + b_1 z + c$$

b_3, b_2, b_1 and c



Model Hyperparameters Definition

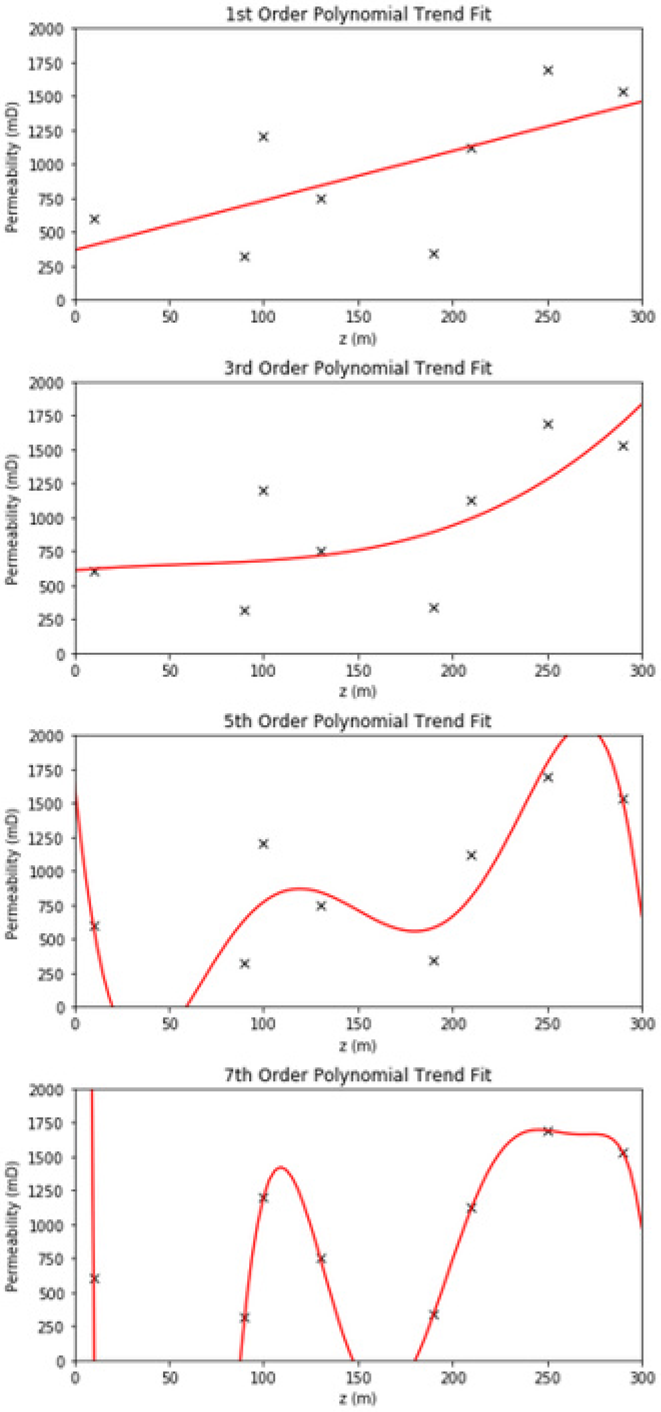
Model Hyperparameters

Set prior to learning from the data. Impact the form of the model and often the complexity.

3rd Order: $$k = b_3 z^3 + b_2 z^2 + b_1 z + c$$

2nd Order: $$k = b_2 z^2 + b_1 z + c$$

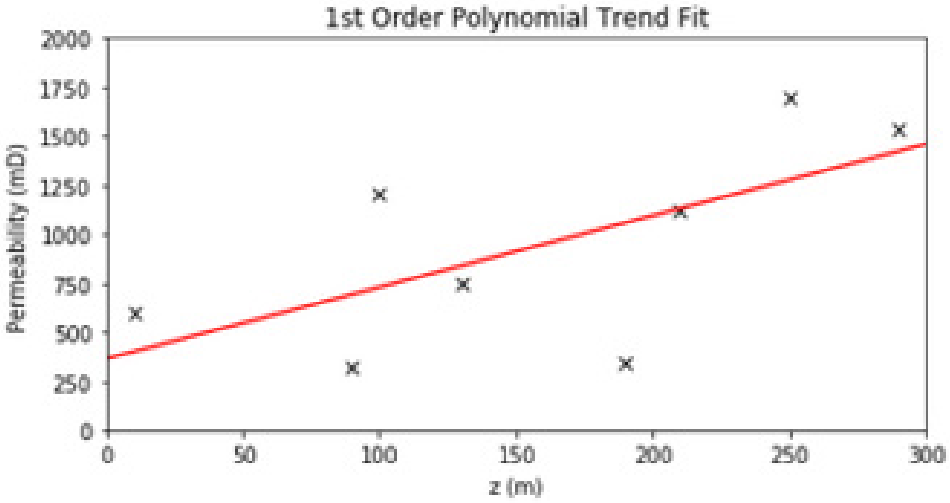
1st Order: $$k = b_1 z + c$$



Prediction Accuracy vs. Model Interpretability / Explainability

Interpretability / Explain-ability

- is the ability to understand the model
- how each predictor is associated with the response
- for example, with a linear model is very easy to observe the influence of each predictor on the response
- but for an artificial neural net it is very difficult



Complexity / Flexibility

Complexity / Flexibility

- Consider these potential polynomials $\hat{f}$ to predict $\hat{Y}$

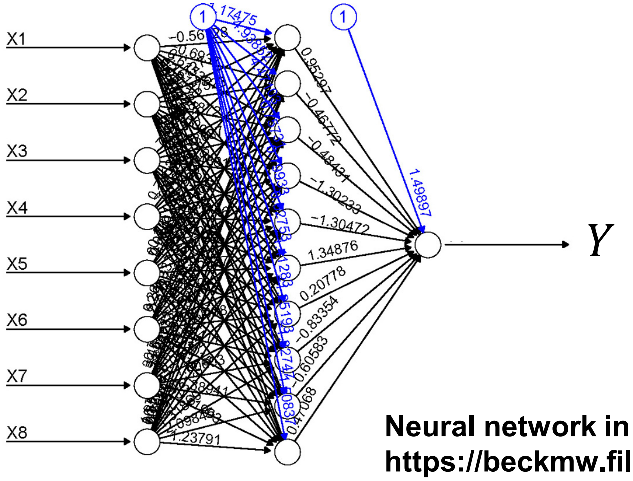
$$Y = \beta_0 + \beta_1 X$$

$$Y = \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 X^3 + \beta_4 X^4 + \beta_5 X^5 + \beta_6 X^6$$

- The 6th order polynomial is more complicated and more flexible to fit the relationship between feature, X, and response, Y
- Now, what if we use 8 bins on X and 10 nodes in a hidden layer of a neural net?:

Indicator Code X into Bins

$$\boldsymbol{I(x; x_k)} = \begin{cases} \boldsymbol{1, if\ x \in\ X_k} \\ \boldsymbol{0, otherwise} \end{cases}$$



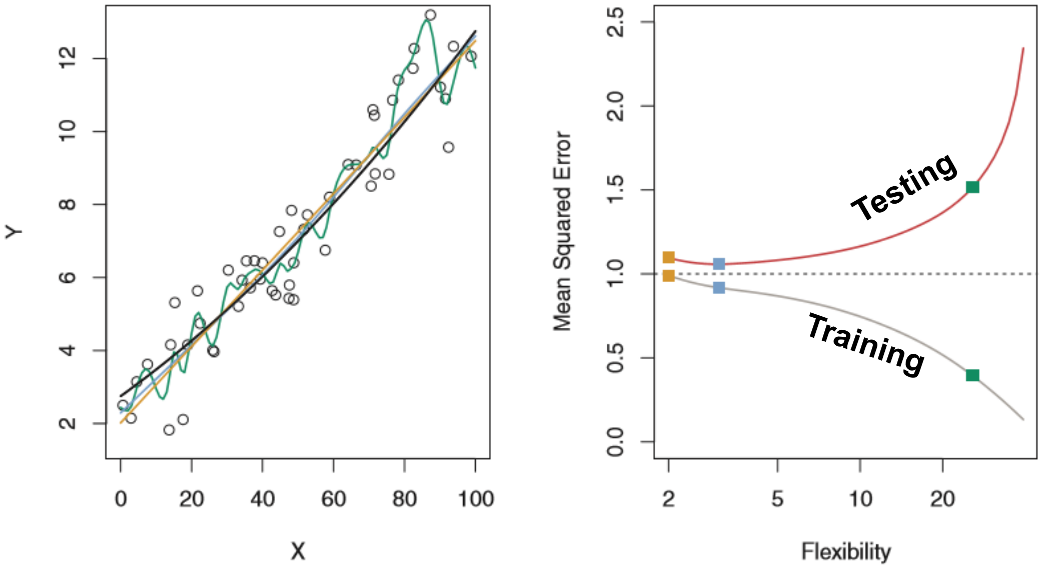
We will discuss neural nets later.

Neural network in R image from: https://beckmw.files.wordpress.com/2013/11/neuralnet_plot.jpg

Assessing Model Accuracy

Flexibility / Complexity vs. Accuracy

- Increased flexibility will generally decrease MSE on the **training dataset**
- May result in increase MSE with **testing data**
- Not generally a good idea to select method only to minimize training MSE



Data and model fits (left) and MSE for training and testing (right) from James et al. (2013).

Bias and Variance Trade-off

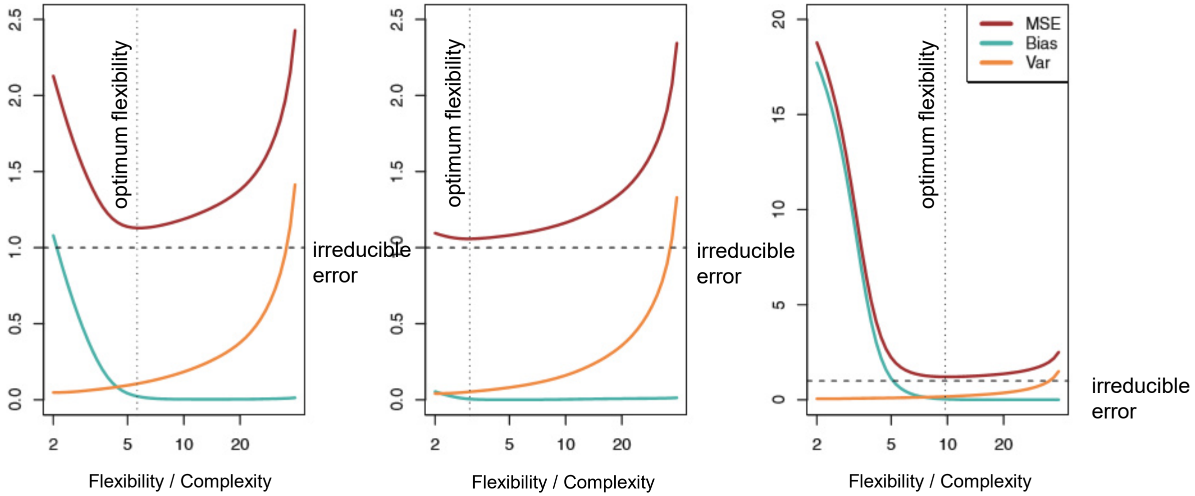
- The **Expected Test Mean Square Error** may be calculated as:

$$\mathrm{E}\left[\left(y_0 - \hat{f}(x_1^0,\dots,x_m^0)\right)^2\right] = \underbrace{Var\left(\hat{f}(x_1^0,\dots,x_m^0)\right)}_{\text{Model Variance}} + \underbrace{\left[Bias\left(\hat{f}(x_1^0,\dots,x_m^0)\right)\right]^2}_{\text{Model Bias}} + \underbrace{Var(\epsilon)}_{\text{Irreducible}}$$

Model Variance is the variance if we had estimated the model with a different training set (simpler models ⇩ lower variance)

Model Bias is error due to using an approximate model (simpler models ⇧ higher bias)

Irreducible error is due to missing variables and limited samples ⇨ can't be fixed with modeling



Model variance, model bias and test MSE for 3 datasets with variable flexibility (Fig 2.12, James et al., 2013), labels added for clarification.

Statistical Learning New Tools

Topic	Application to Subsurface Modeling
Data Analytics is the use of statistics, geoscience and engineering with data.	Learn applied statistics and workflows to support your work with data. *Growing new competencies to augment geoscience and engineering expertise is a great solution, consider open source packages in Python.*
Parametric and Nonparametric	Parametric models need less data to train but may have model bias, nonparametric models often are parametric rich and may be overfit. *Be aware of the performance of your selected modeling methods.*
Model bias, Model variance and Irreducible Error	There is an error trade-off for accuracy with testing data. *Low complexity models may outperform high complexity models.*

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