Biostat 202: Opportunities and Challenges of "Big Data": Machine Learning 1: Regression

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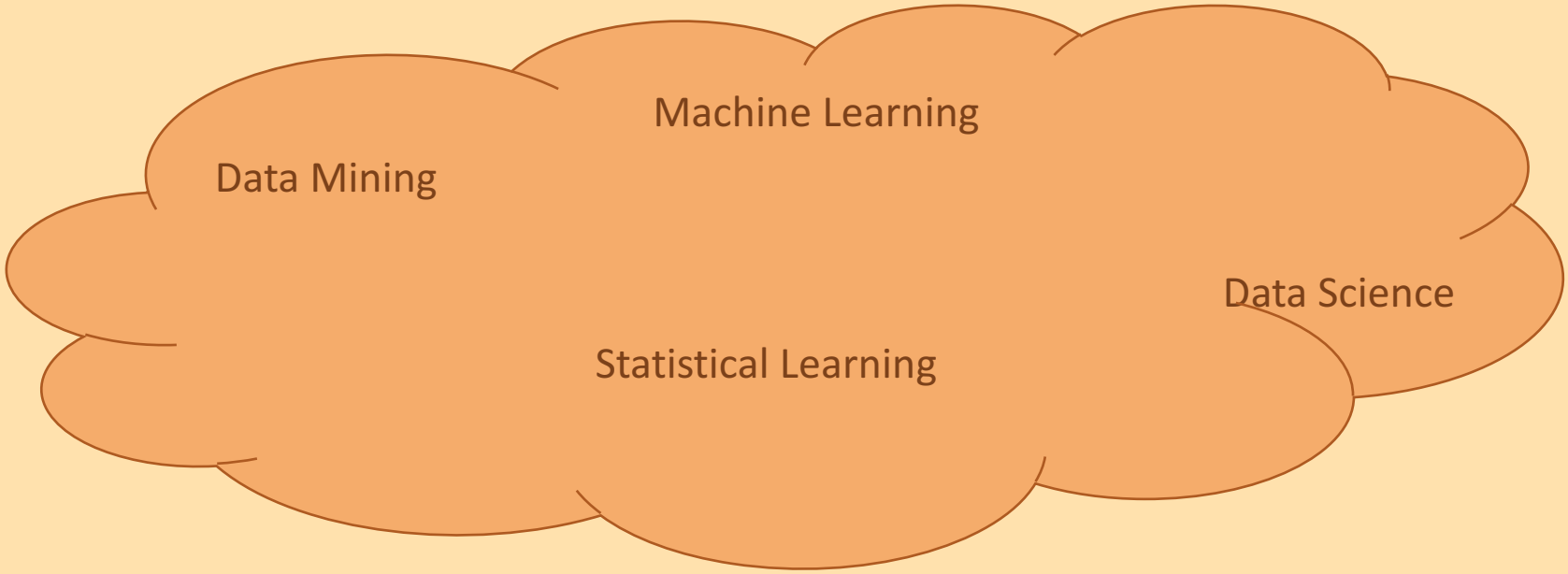
Overview of machine learning lectures

- 4 lectures
- Machine Learning “definition”
- Supervised vs. unsupervised Machine Learning
- Regression (supervised prediction)
- Classification (supervised prediction)
- Validation and testing
- Cross-validation
- Bagging and boosting
- Clustering (unsupervised)
- Data reduction techniques (unsupervised)
- IBM SPSS Data Modeler examples throughout

Overview of this lecture

- Machine Learning and the big picture
- Supervised vs. Unsupervised Machine Learning
- Prediction using:
  - Linear regression
  - Multiple regression
- Validation

Machine Learning?



Machine learning

- *Machine learning* is a subfield of computer science that evolved from the study of pattern recognition and computational learning theory in artificial intelligence. In 1959, Arthur Samuel defined machine learning as a "Field of study that gives computers the ability to learn without being explicitly programmed"

- *Machine learning* is a type of artificial intelligence (AI) that provides computers with the ability to learn without being explicitly programmed. Machine learning focuses on the development of computer programs that can teach themselves to grow and change when exposed to new data.

- We are not trying to create AI, but rather use some machine learning algorithms for the purpose of prediction or identifying patterns in data.

Supervised vs unsupervised

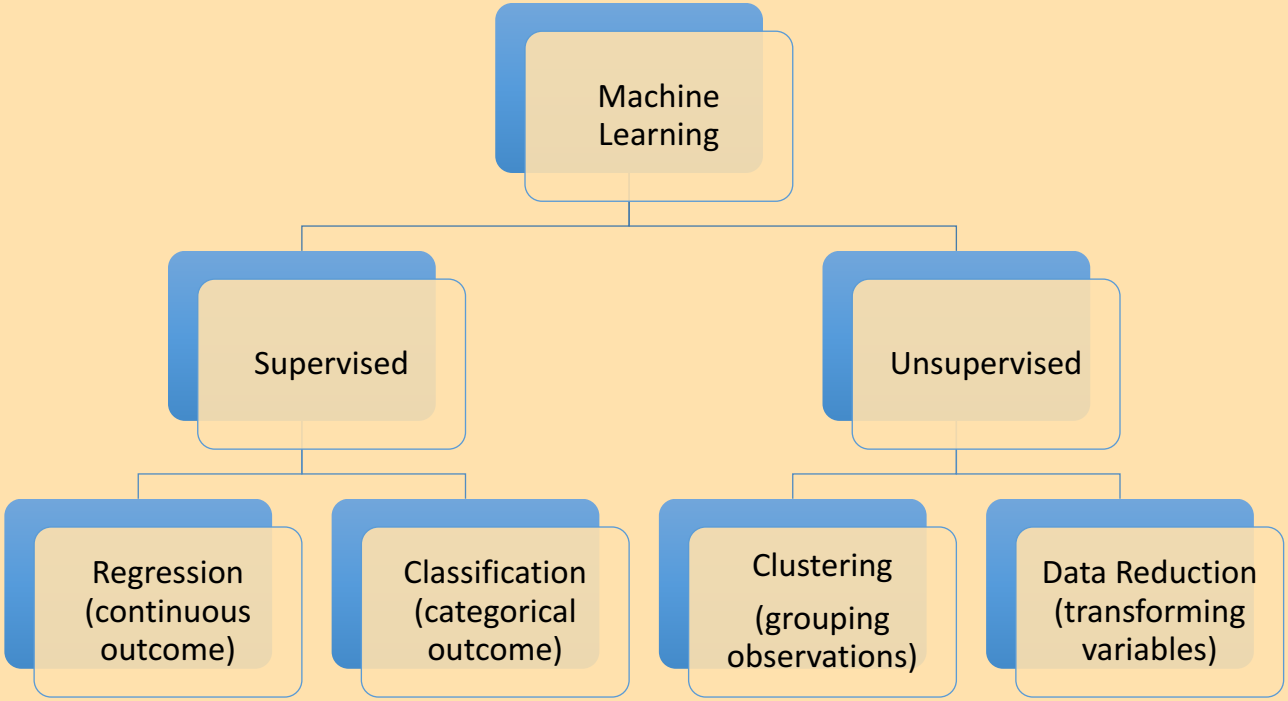
- **Supervised Learning**
- Have data where you know outcome in order to *train* the model
- Train the model to predict future outcomes from sets of predictors

Prediction: Regression (continuous outcomes) and classification (categorical outcomes)

- **Unsupervised Learning**
- No specified outcomes
- Separate data points into groups with "similar" properties (clustering)
- Or reduce data to fewer variables in some way that still captures important structure of the data

Clustering and data reduction

Supervised vs. unsupervised



Prediction problems

- Predict the CD4 count in a patient 6 months from now based on current CD4, viral load, demographic and lifestyle variables
- Predict whether a patient will develop breast cancer based on genetic, demographic, and lifestyle variables
- Predict whether or not, and what type of dementia a patient has based on MRI of the brain (a running example for these lectures)

Definitions

- *Instance* (also *Item*, *Record*) = observation:
  - an example, described by a number of attributes,
  - e.g. a day can be described by temperature, humidity and cloud status
  - e.g. a person can be described by age, gender, blood pressure and level of physical activity
- *Attribute* or *Field* = variable
  - measuring aspects of the Instance, e.g. temperature
- *Class* or *Label* = class or group
  - grouping of instances/observations, e.g. disease type

Definitions

- *Target*. Also called *outcome*, *response*, *dependent variable* – the variable that you want to predict
- *Input*. Also called *predictor*, *covariate*, *independent variable* – the variables you will use to predict
- Modeler also has variable roles of *Record ID* (identification variable like medical record number), *split* (for separate analyses of subgroups), and *partition* (for assessing training/testing).

Regression

- Start simple with one predictor
- We will move onto multiple predictors later…

Linear Regression

Consider a response variable y as linearly related to an attribute/predictor x, then:

$$y = ax + c$$

e.g. y = Systolic BP (SysBP)

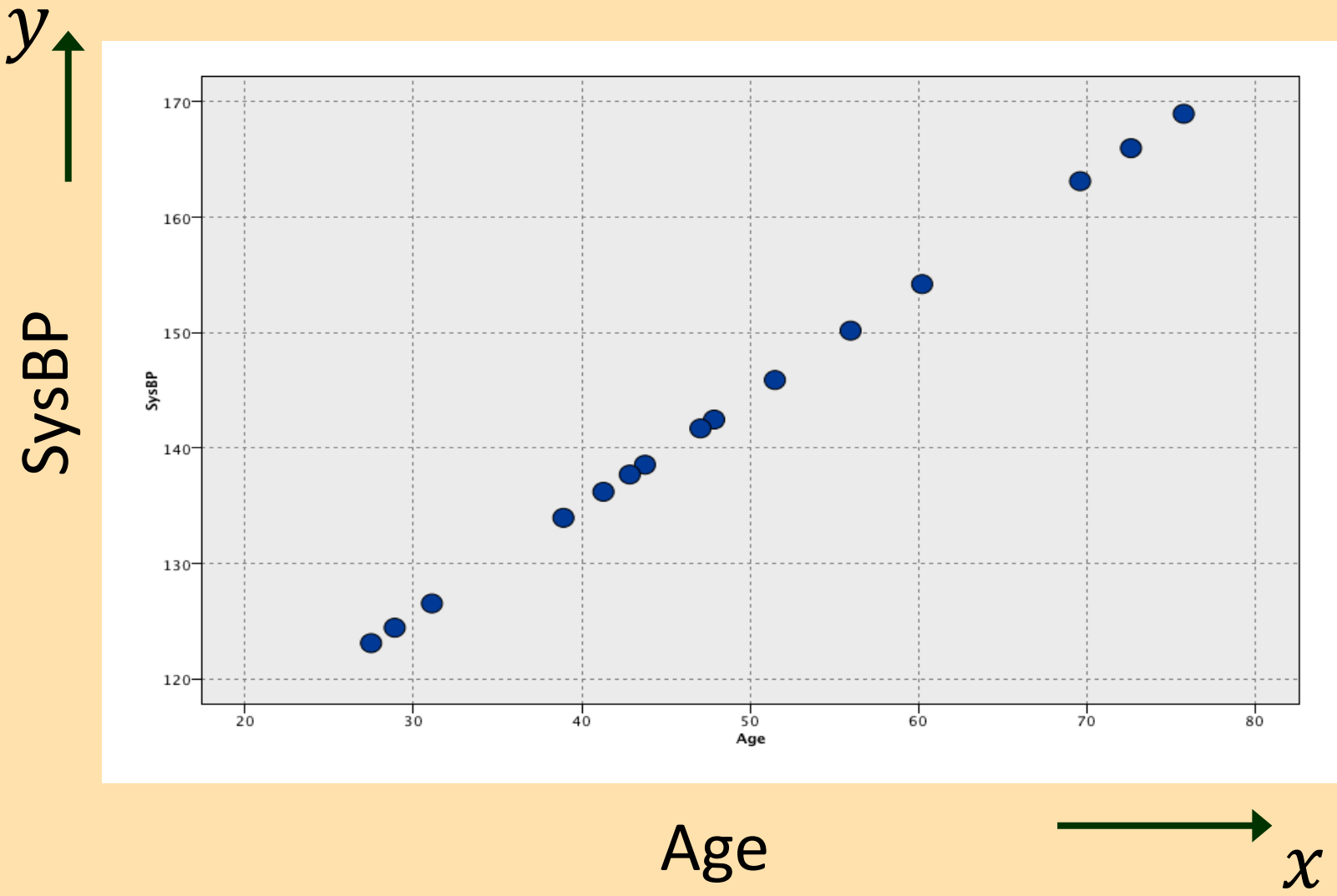
x = Age

c = intercept (SysBP at age 0)

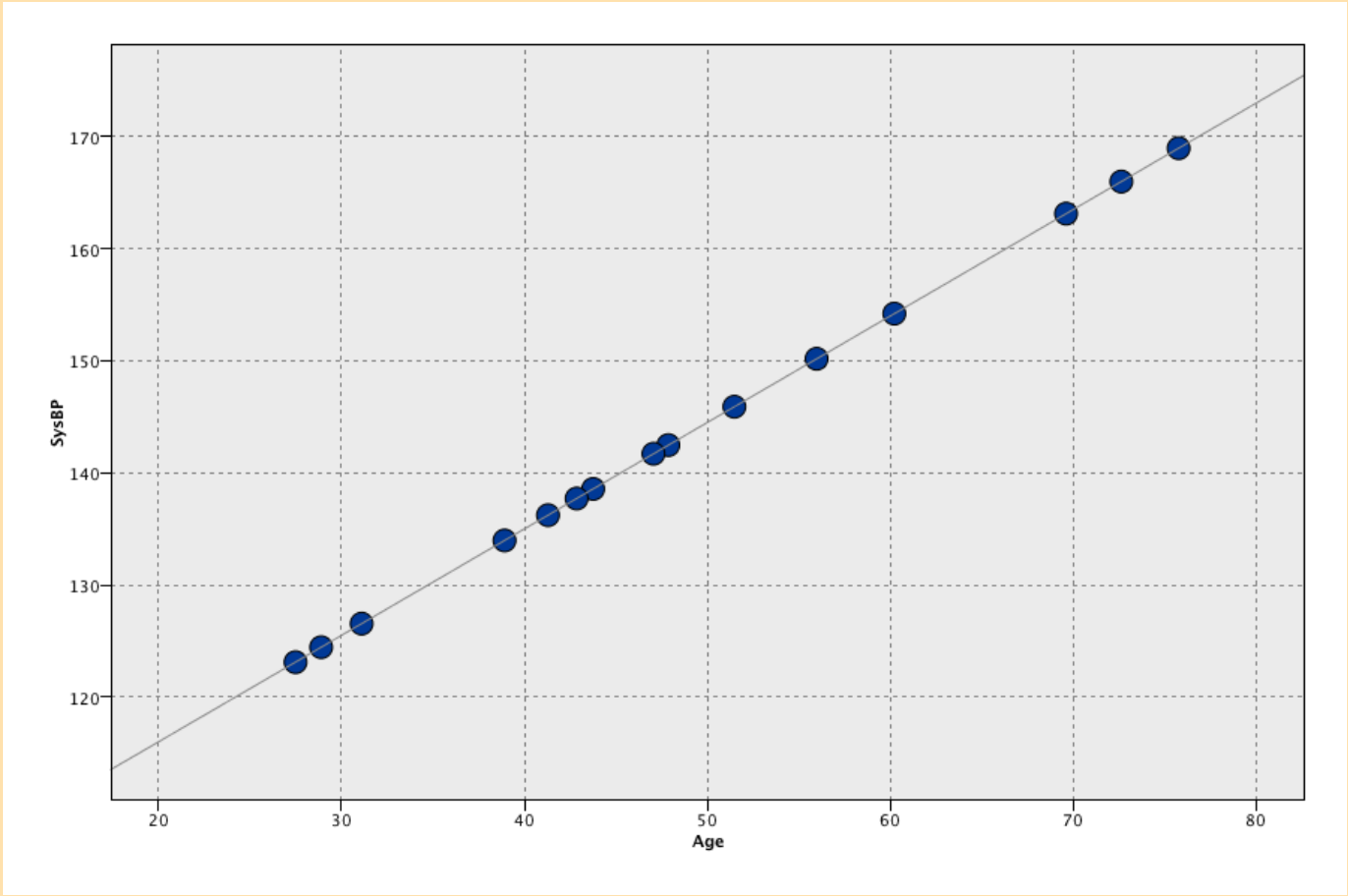
a = change SysBP per year in Age

Question: Is Age predictive of SysBP?

Fitting linear regression



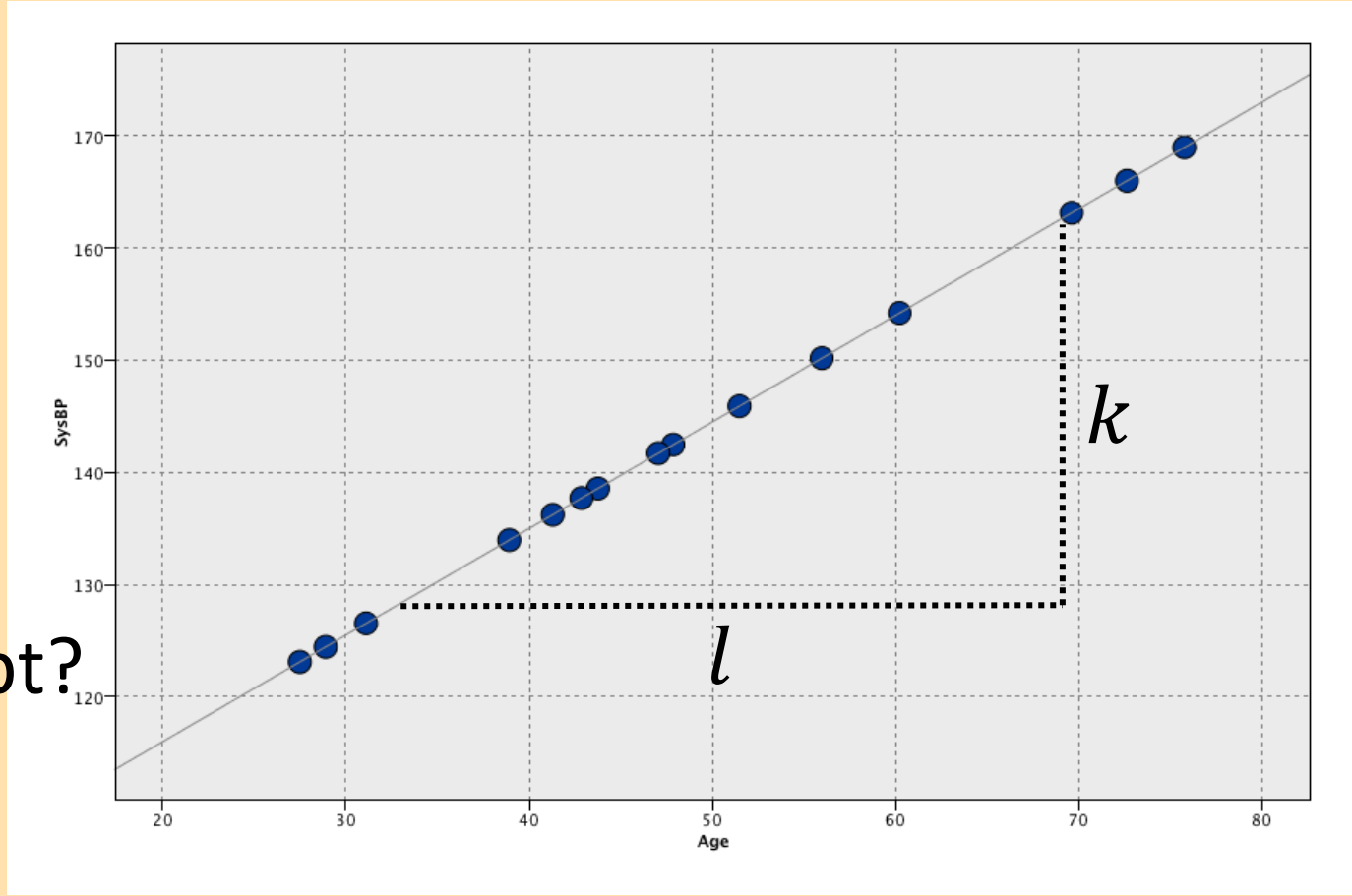
Fitting linear regression



Fitting linear regression

y

SysBP



slope

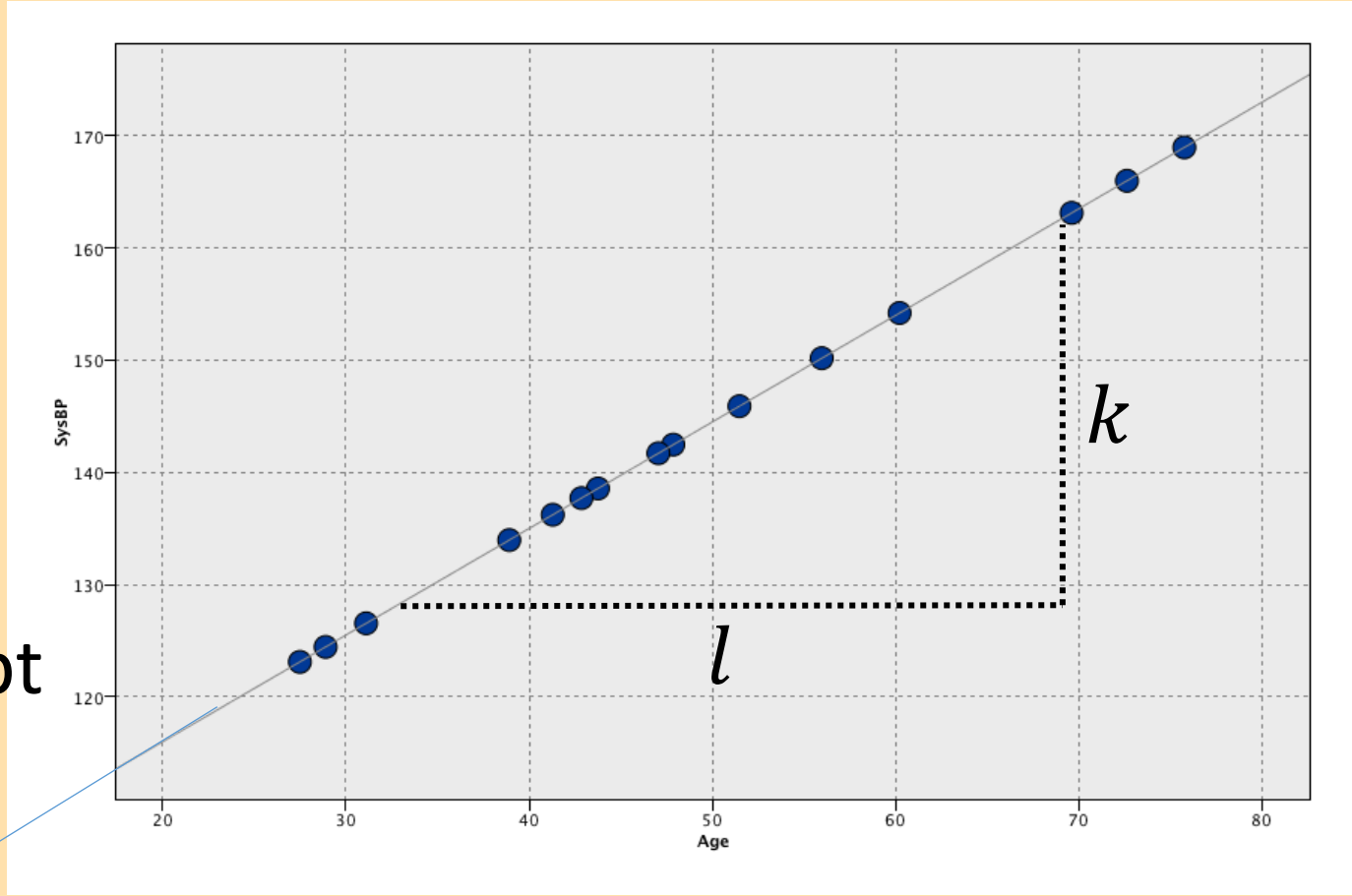
$$a = \frac{k}{l}$$

Intercept?

Age

x

Fitting linear regression

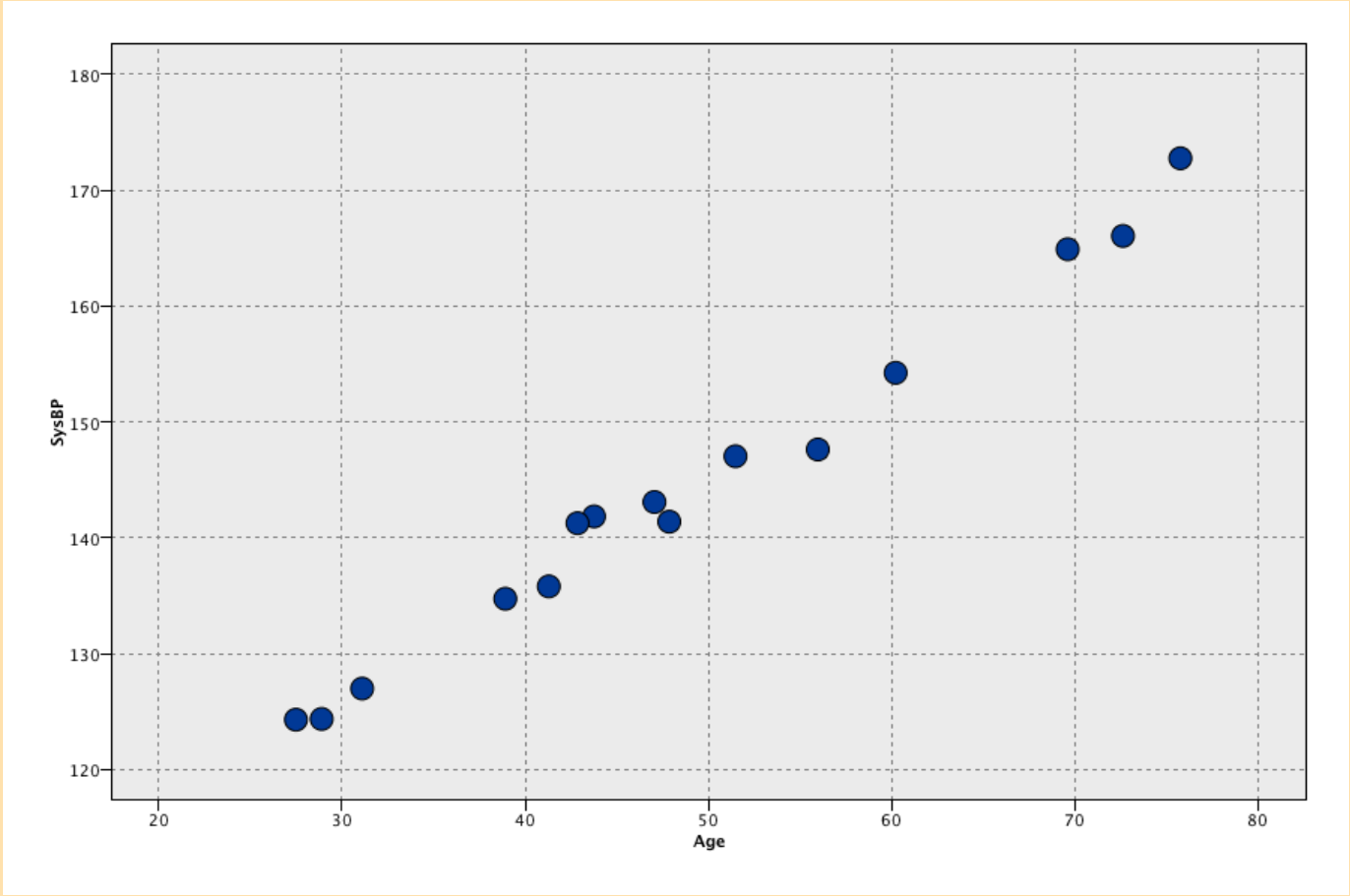


Fitting linear regression

- But data (almost) never lie on a perfect straight line. The data also contain:
  1. Measurement error
  2. Between subject variability (e.g. not all people of a certain age have the same Systolic BP)

Data with measurement error

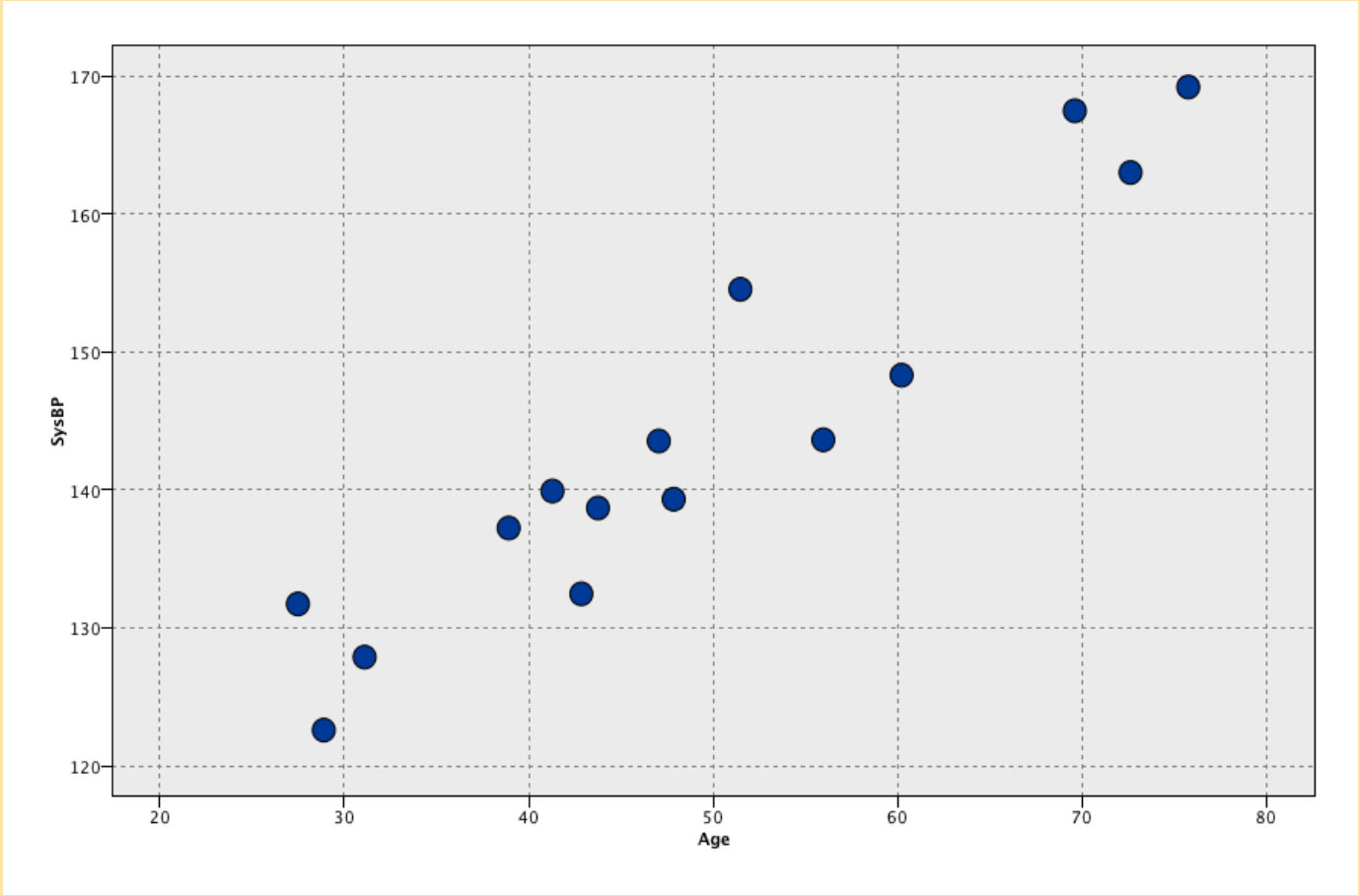
SysBP



Age

Data with measurement error plus biological variability

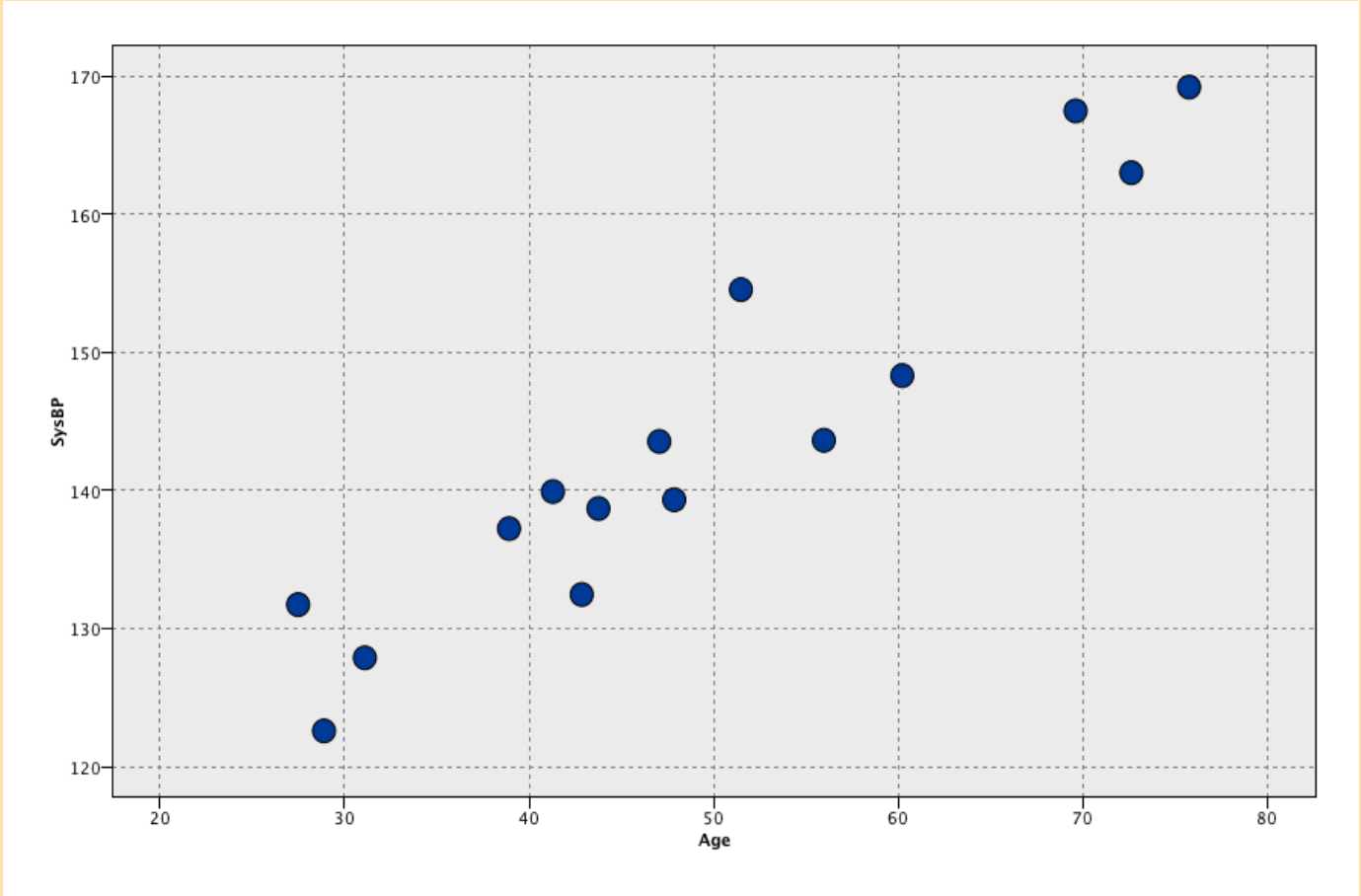
SysBP



Age

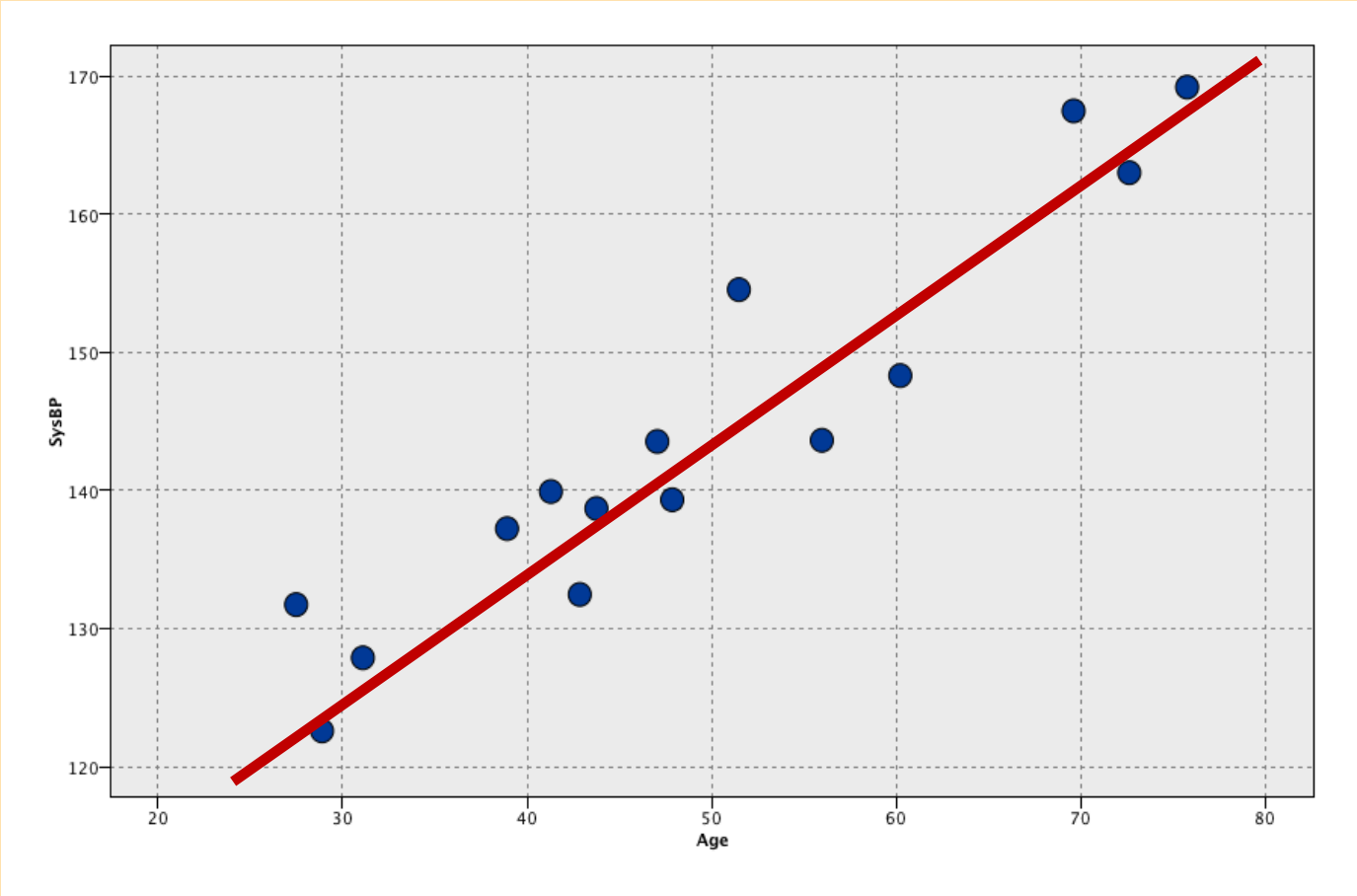
How to choose a fitted line?

SysBP



Age

How to choose a fitted line?



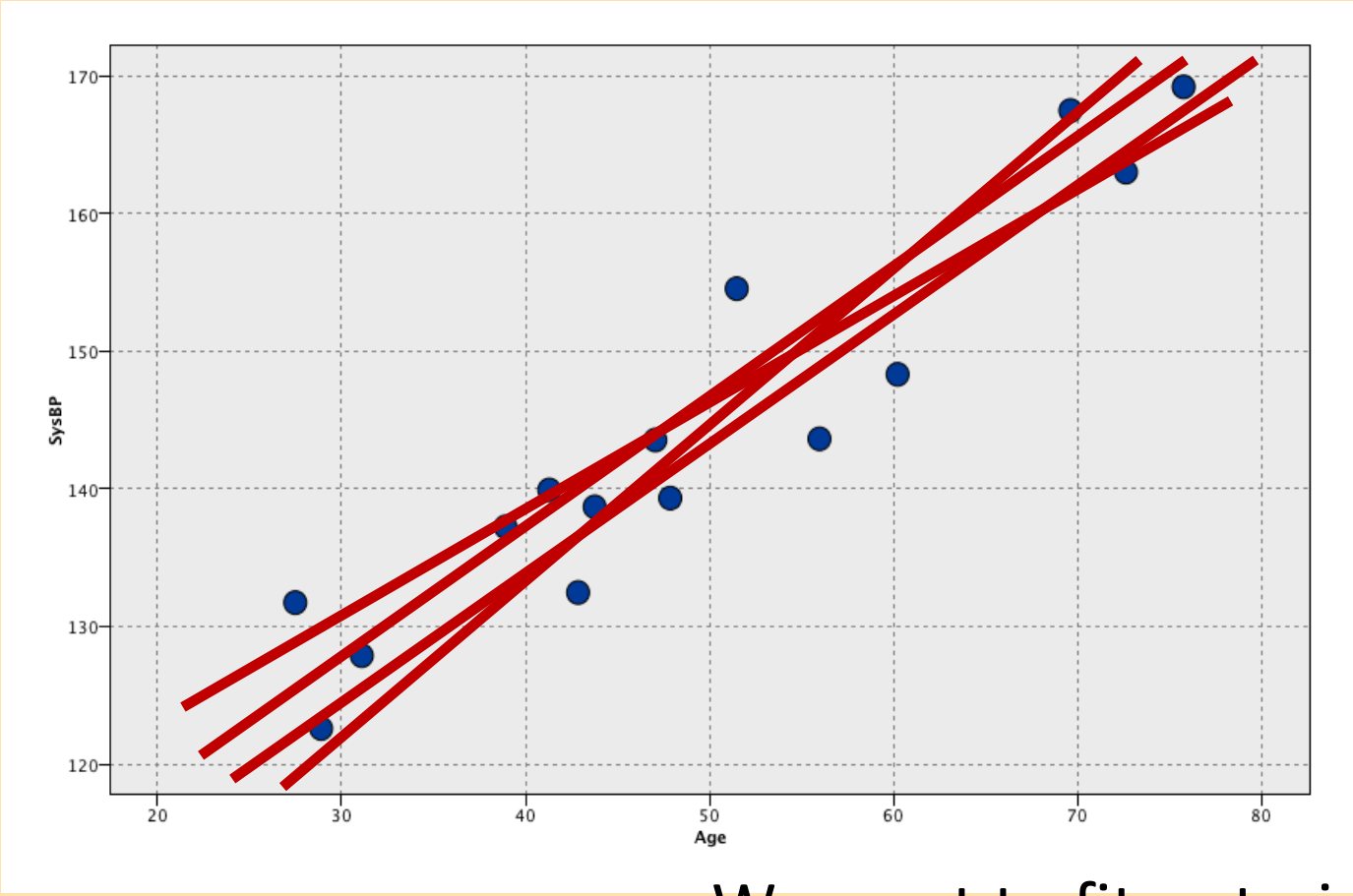
SysBP

Age

One possible line

How to choose a fitted line?

SysBP

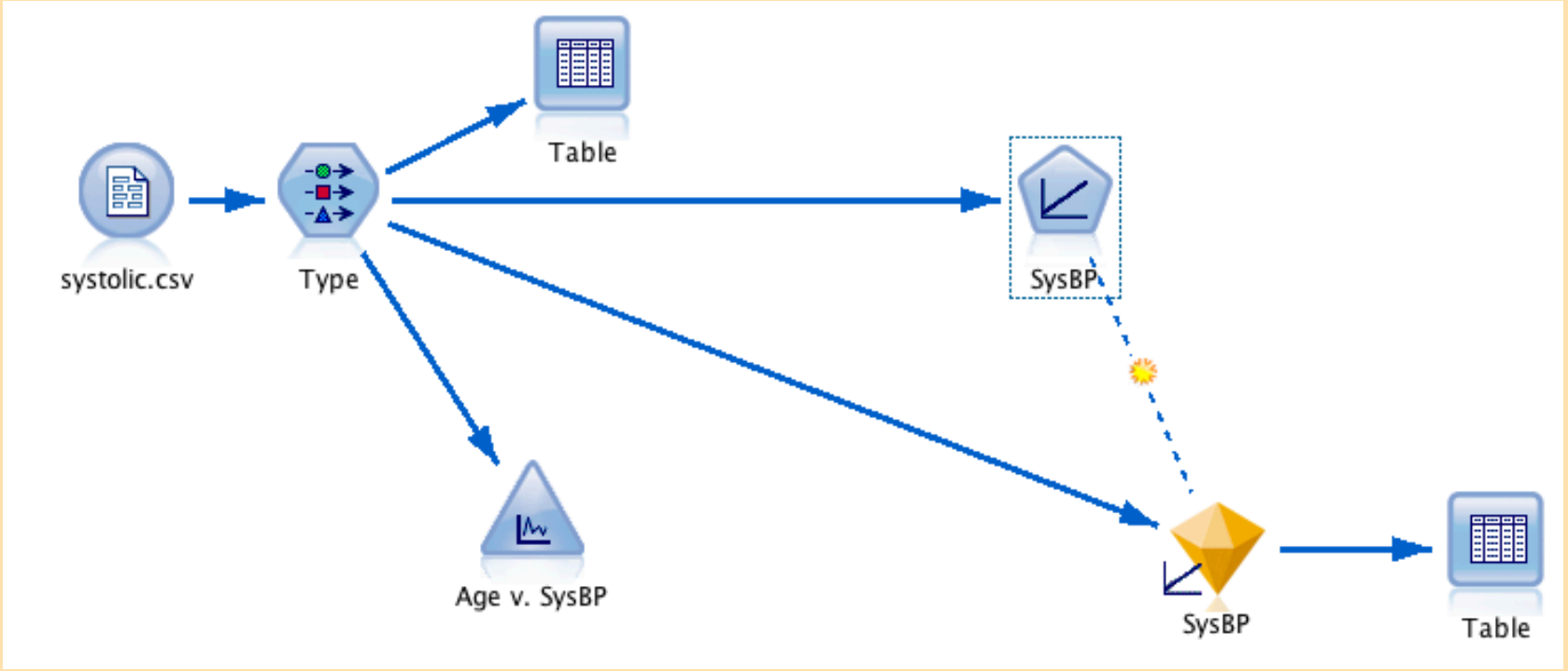


Age

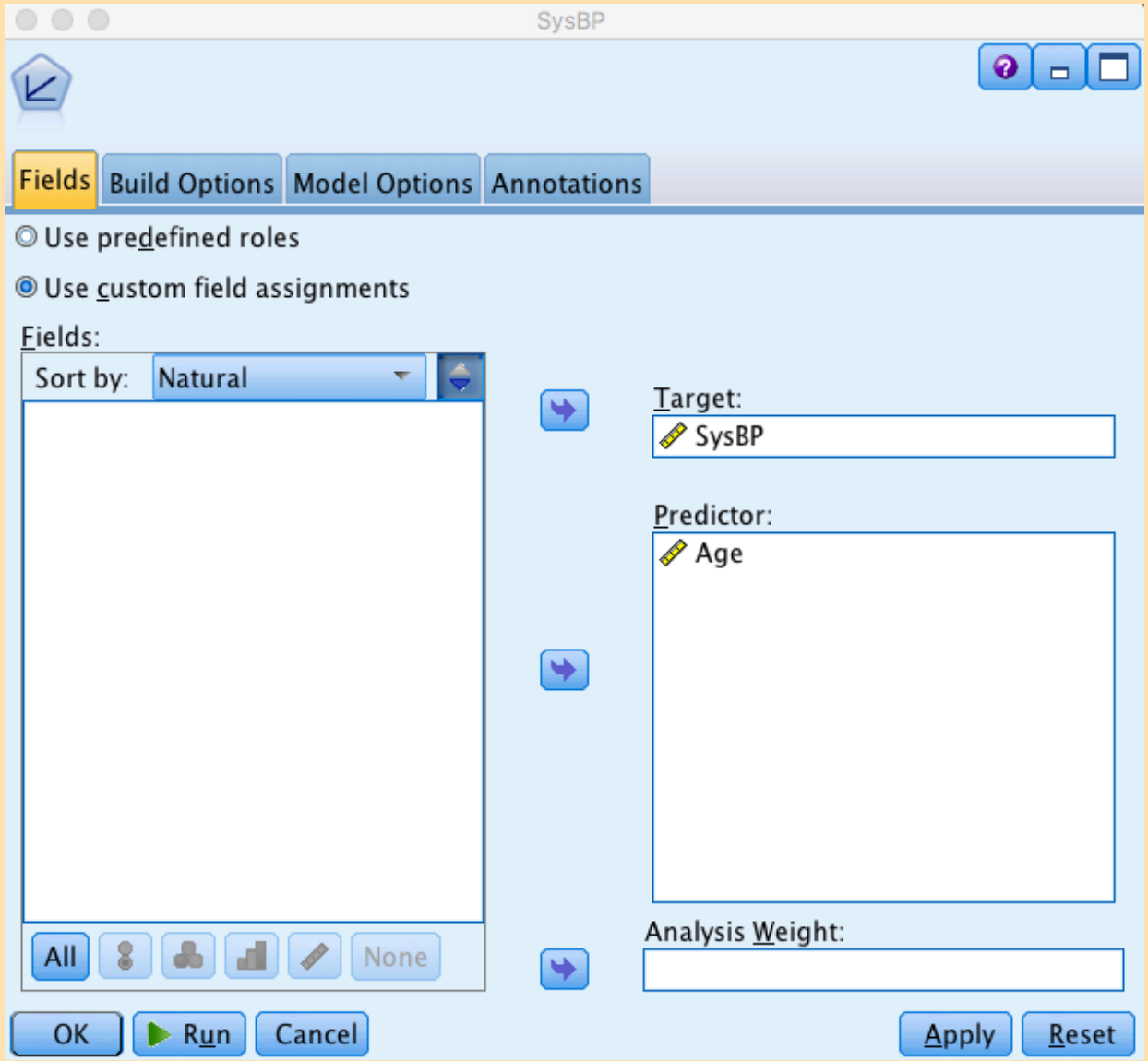
We want to fit a straight line to give us a relationship, but which one is ‘best’?

IBM Modeler linear regression stream

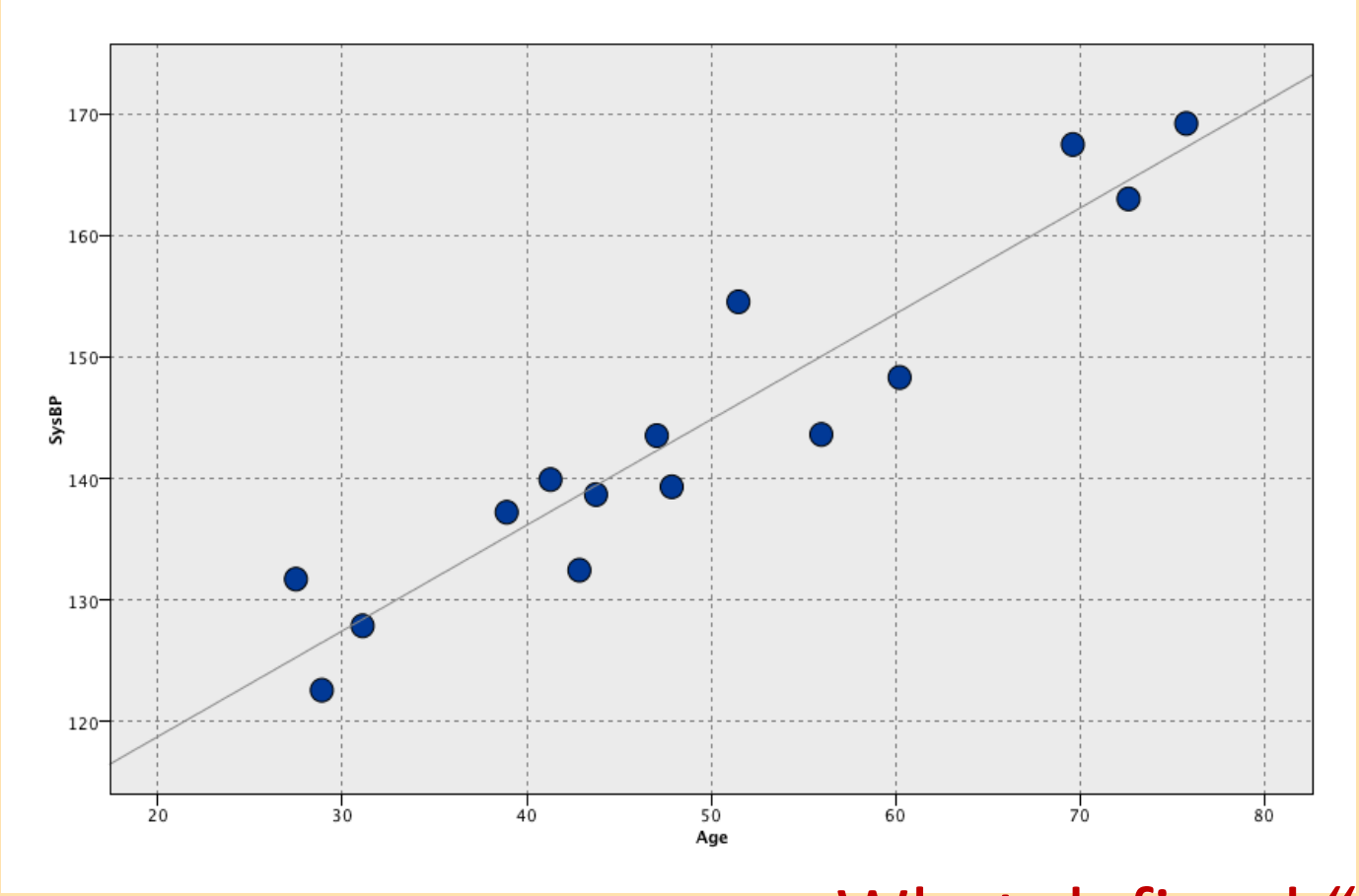
Modeling tab



IBM Modeler Linear Node



Fitted line from Linear node



SysBP

Age

What defined “best”?

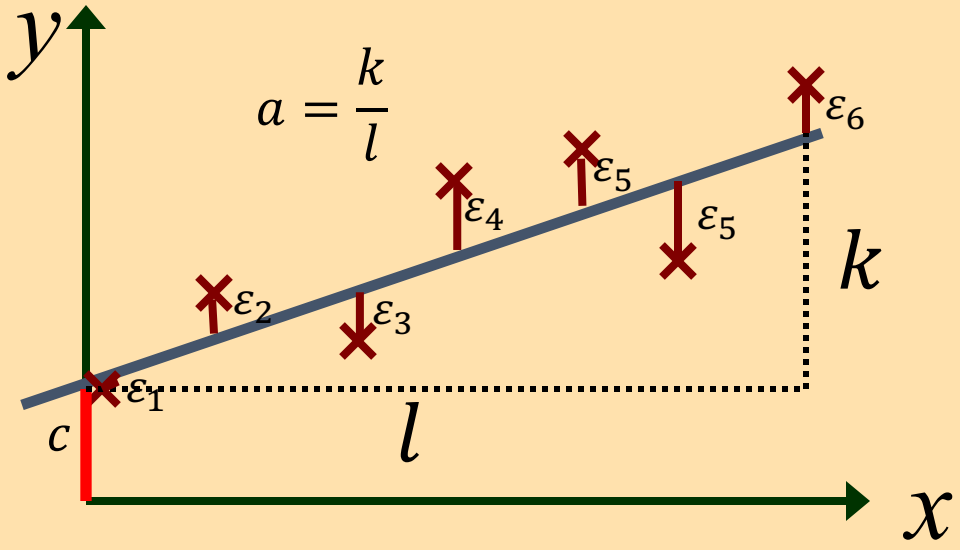
Model Fitting

- Classical statistical models are conventionally fit by a method called *maximum likelihood*
- Equivalent to *least squares fitting* for linear regression/model

  Find the line such that the sum of all the square vertical distances from data points to the line is minimized (see next slide)
- Classical statistical inference focuses on the regression relationship between x and y -- usually concerned with whether there is evidence that the slope a is non-zero and what is its estimated value (and uncertainty)?
- In statistical/machine learning *emphasis* is more on using estimates of a and c to predict future values of y from future values of x -- interested in predictors that add predictive value, not evidence for non-zero relationship

Least Squares

- Model relationship between x and y (e.g. linear)
- Assume error is in y, not in x
- Find the line such that it gives you the smallest *sum of squared* errors

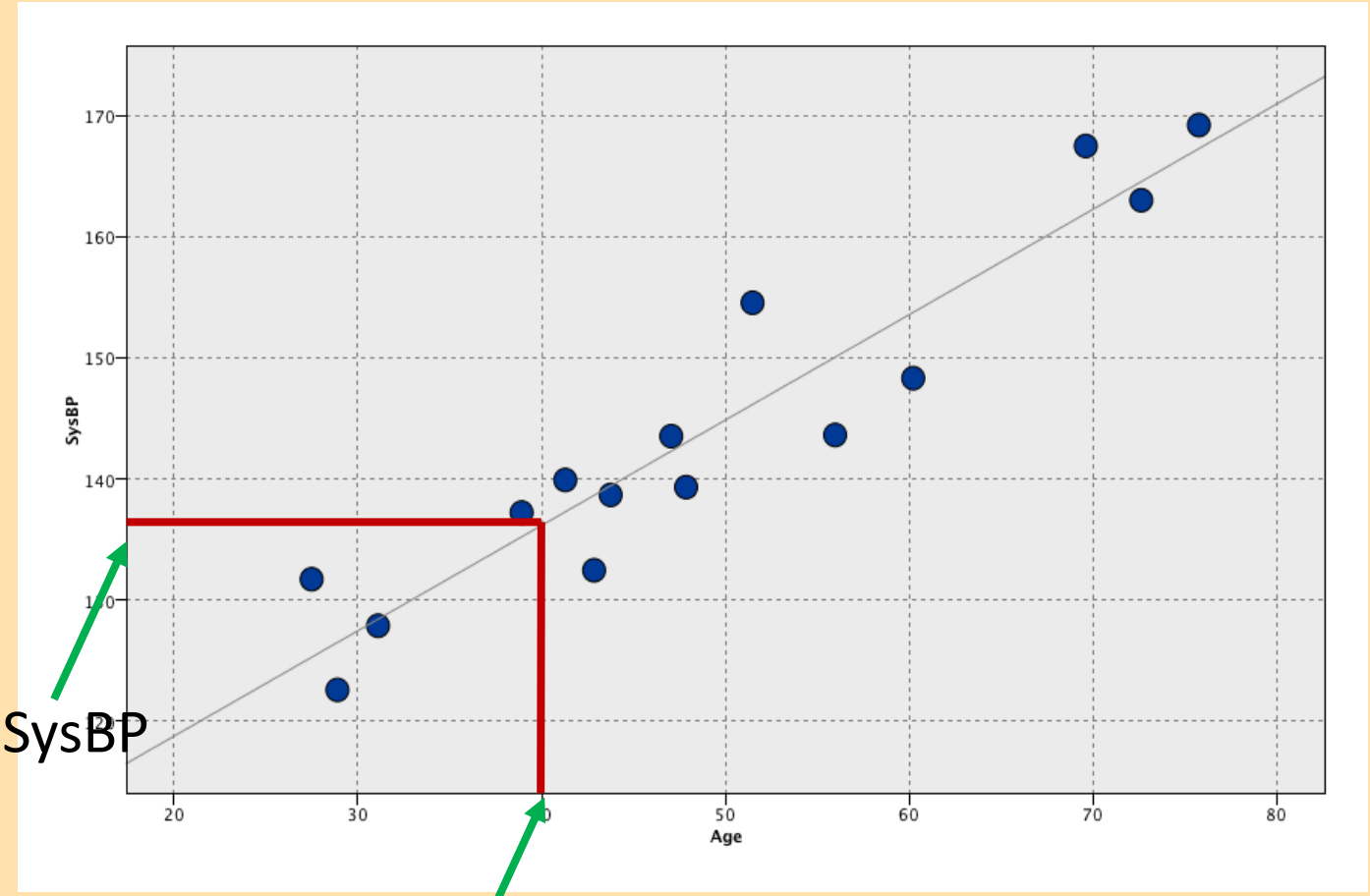


Add the squared values of the vertical red lines together:

$$SS = \varepsilon_1^2 + \varepsilon_2^2 + \varepsilon_3^2 + \varepsilon_4^2 + \varepsilon_5^2 + \varepsilon_6^2$$

choose line that minimizes this total SS

Making a prediction



SysBP

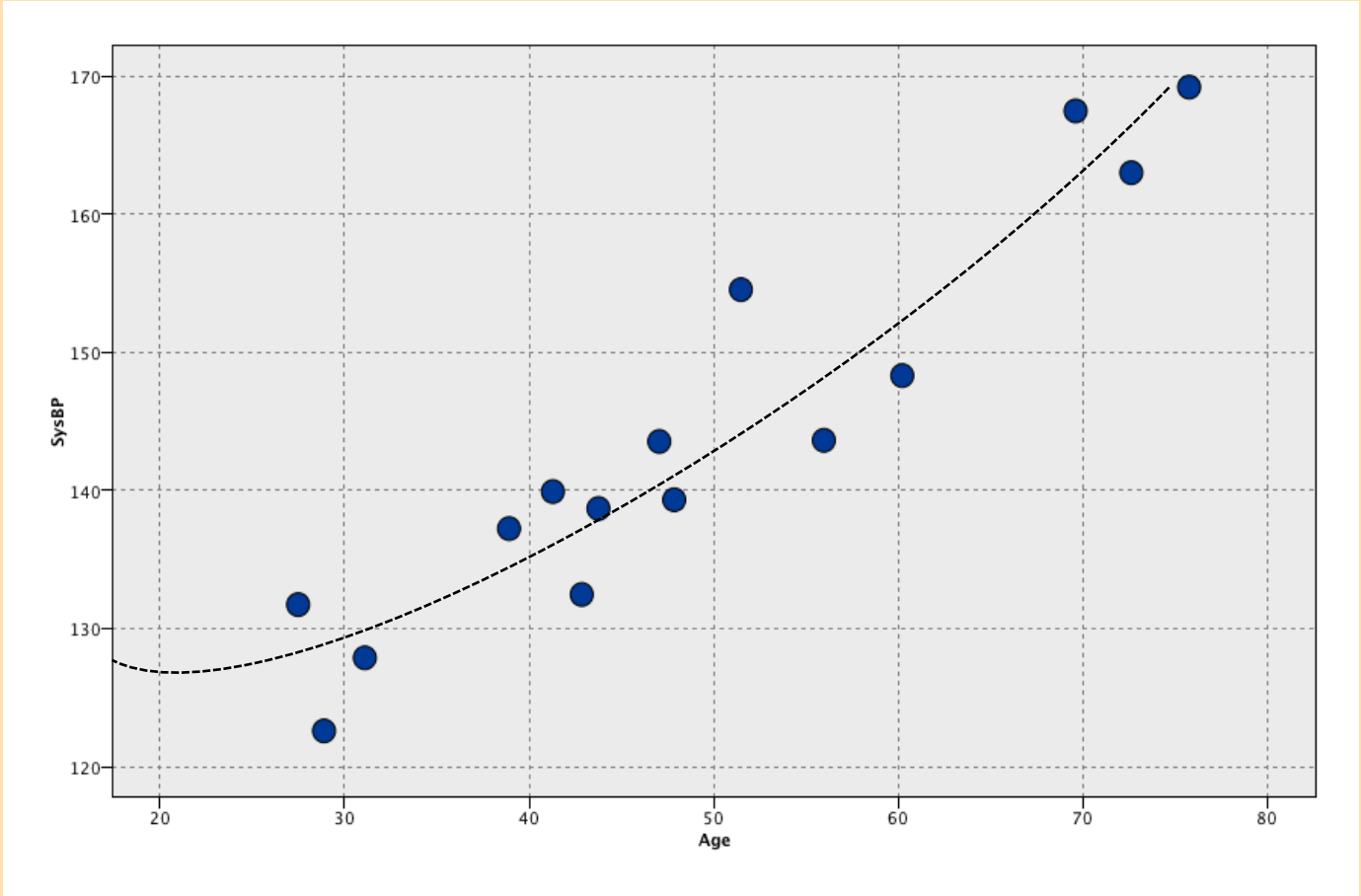
Predicted SysBP

New subject age 40

Age

Why straight line? What about?

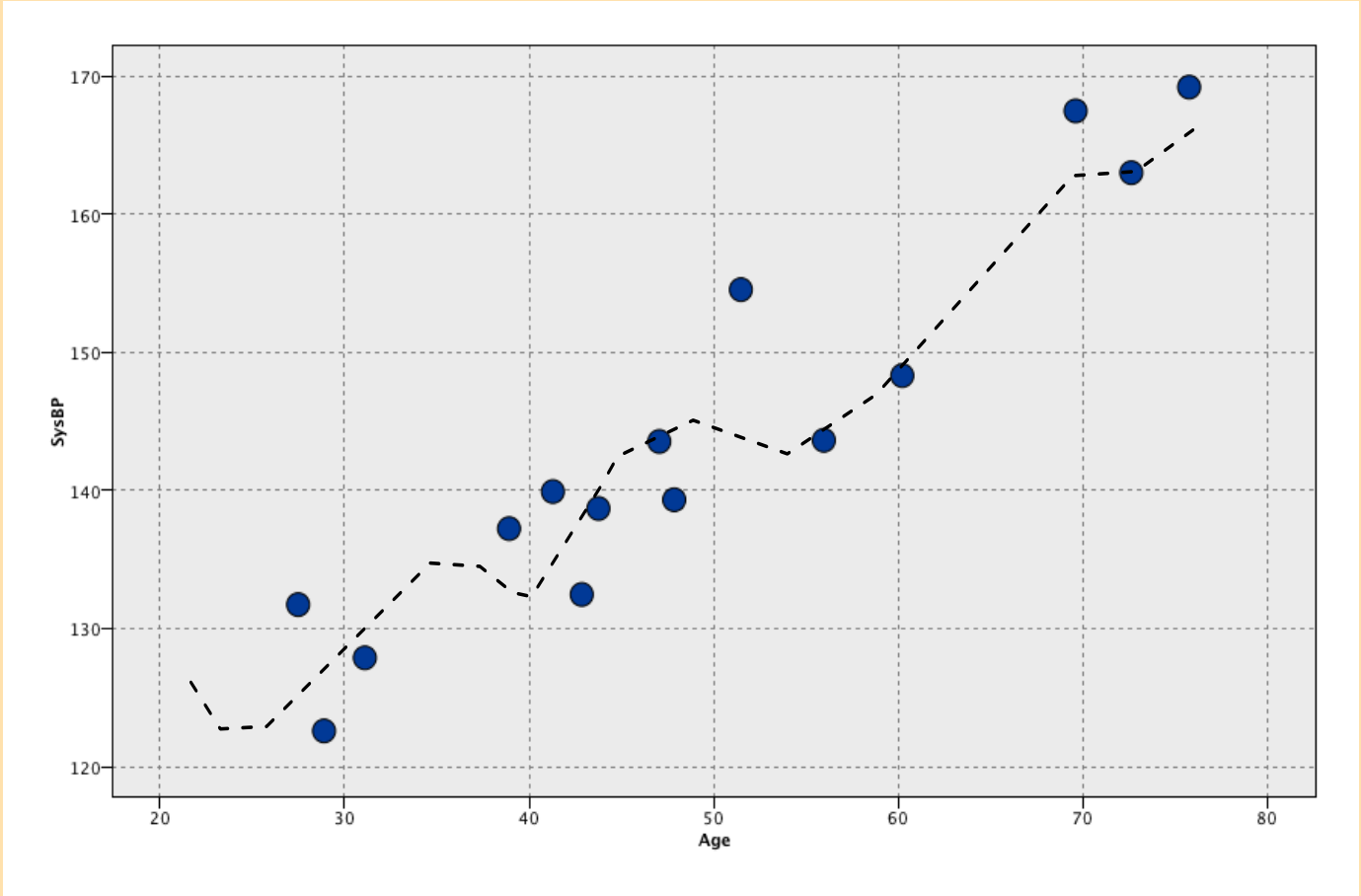
SysBP



Age

Or even?

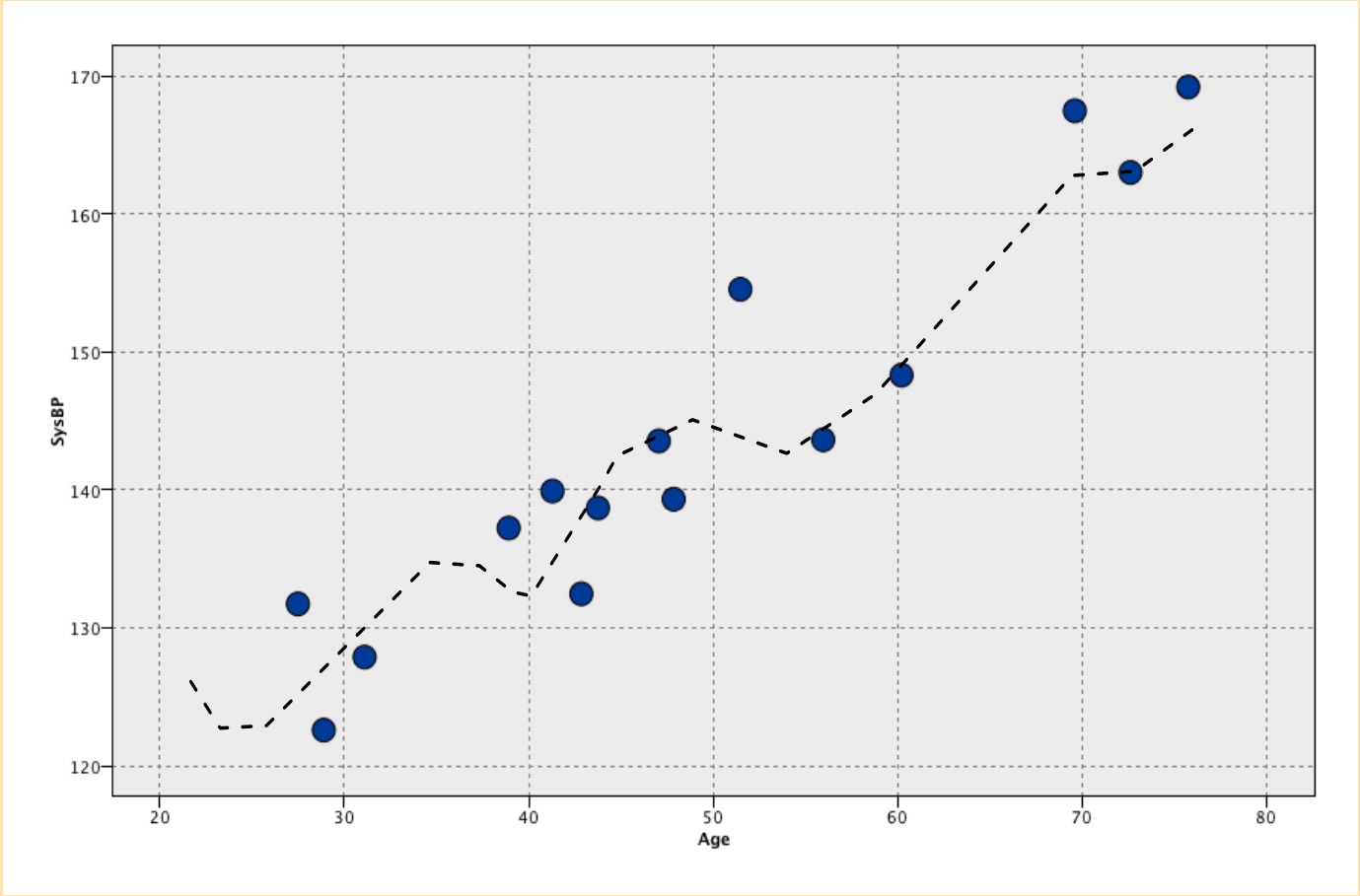
SysBP



Age

Or even?

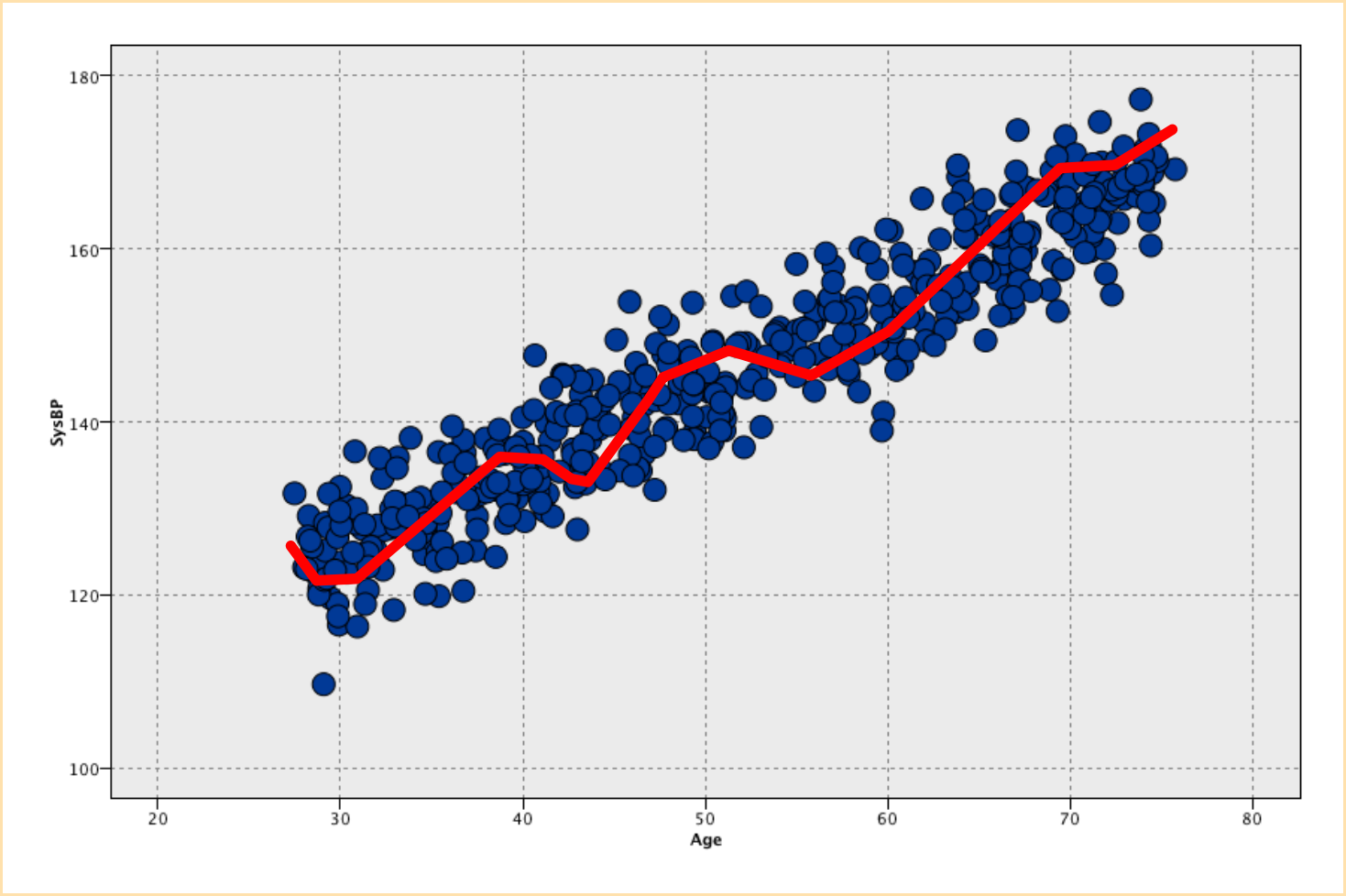
SysBP



Age

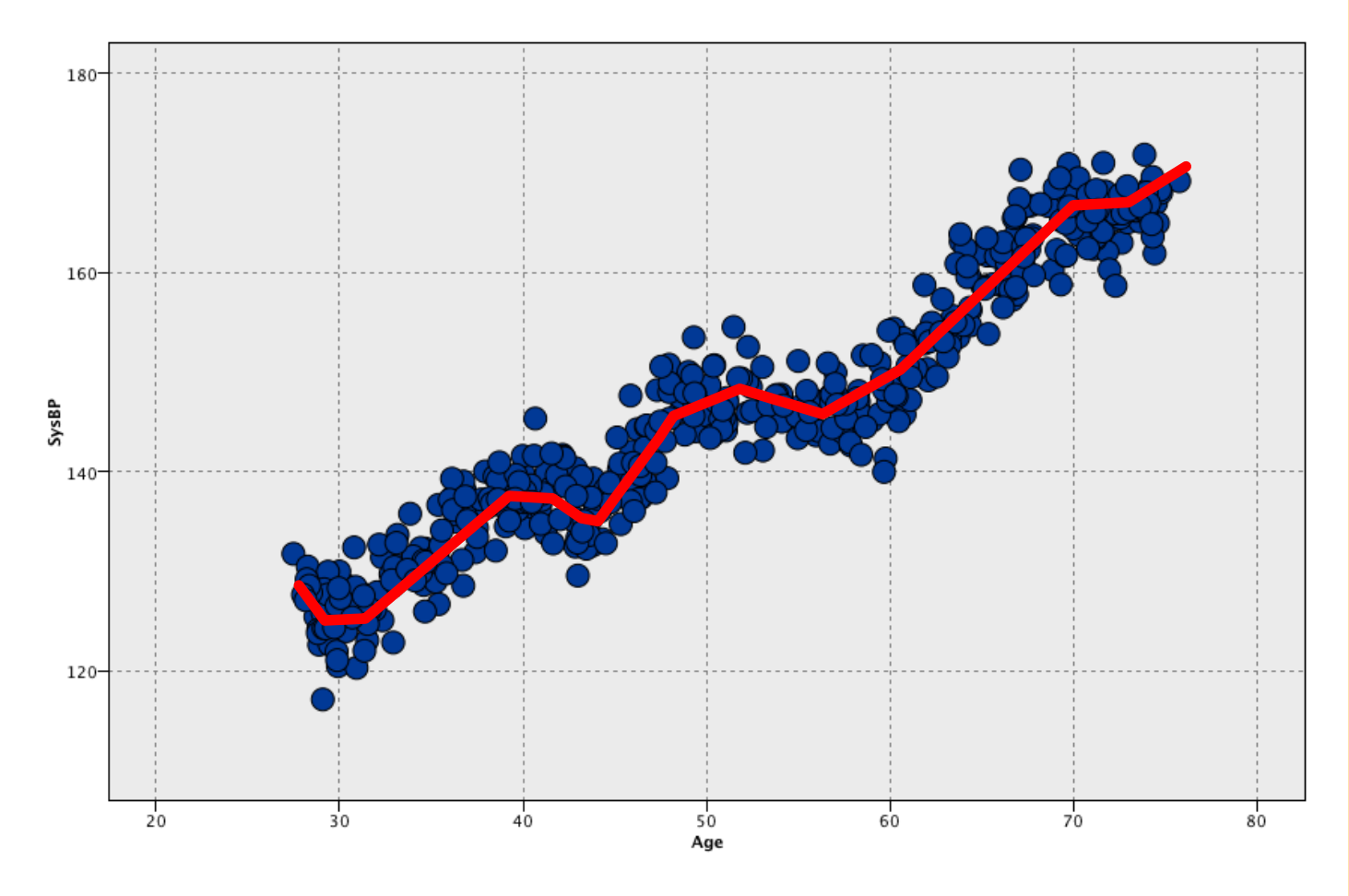
Overfitted?

What about with more data?



What about this data?

SysBP



Age

Big Data – Large N and Large P

- Big data can be thought of in two ways
- Large N = large number of subjects – implies more information for fitting complex models or ones with many predictors
- Large P = large number of predictors, or complex relationships between predictor and outcome, or between predictors (interaction terms)

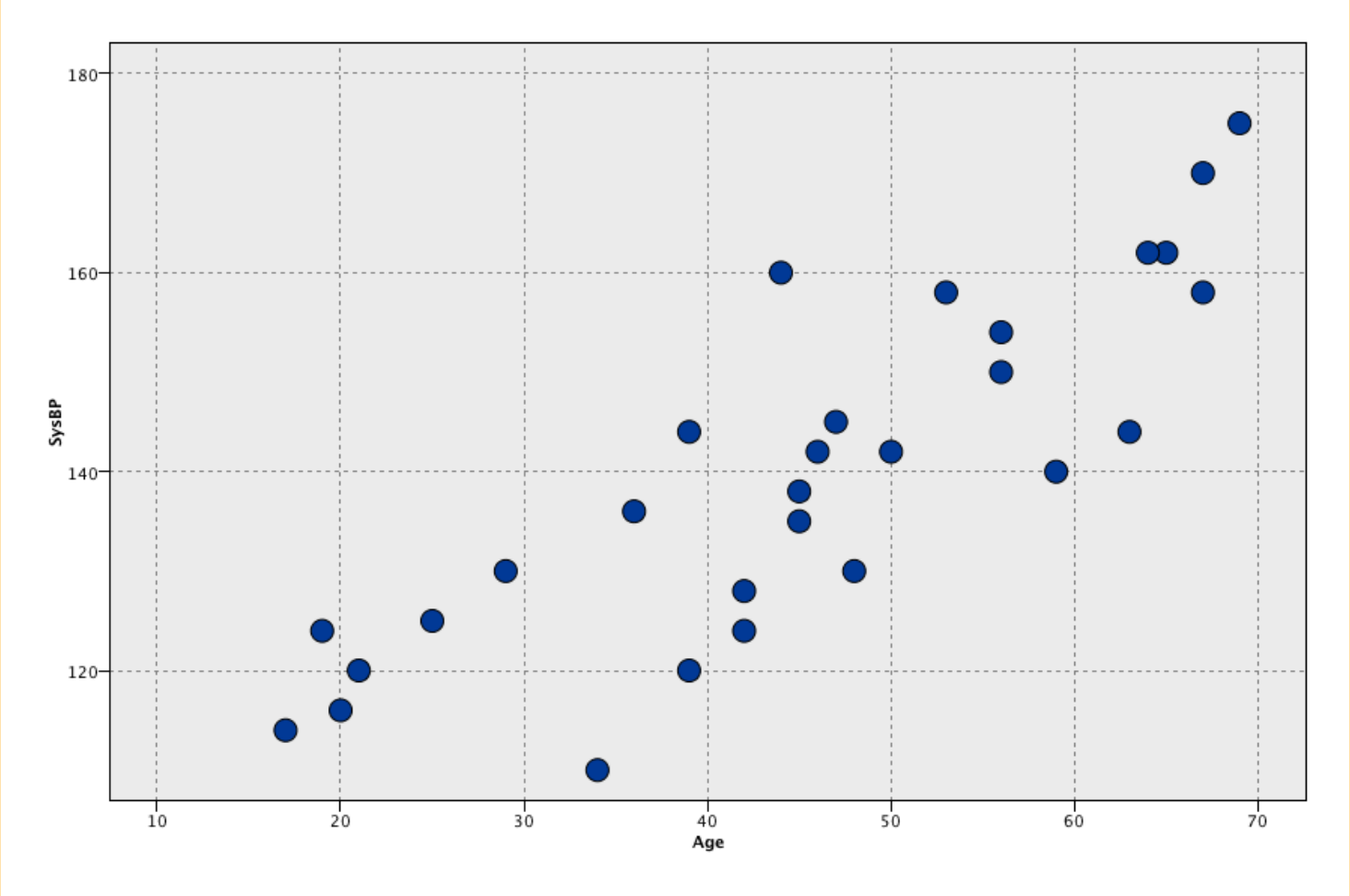
The trade-off for more complex models

- Want to find “true” predictive patterns in the data
- Idea is to use some measure of external “prediction quality” (e.g. least squares) in order to assess what level of complexity is best given a particular dataset
- Want to avoid overfitting spurious detail: i.e. don’t want to make the model capture apparent patterns due to noise, but we want to capture true underlying patterns
- Solution – independent validation – reserve some data that has not been used in model fitting for the purpose of model evaluation and comparison – we will look at this briefly later, and in more detail on Thursday

The SysBP dataset example

- Helmut Spaeth, Mathematical Algorithms for Linear Regression, Academic Press, 1991, page 304, ISBN 0-12-656460-4.
- Data available at: http://people.sc.fsu.edu/~jburkardt/datasets/regression/regression.html as the x03.txt dataset
- I have put Modeler friendly version on CLE
- The systolic blood pressure was measured for 30 people of different ages.

The SysBP dataset

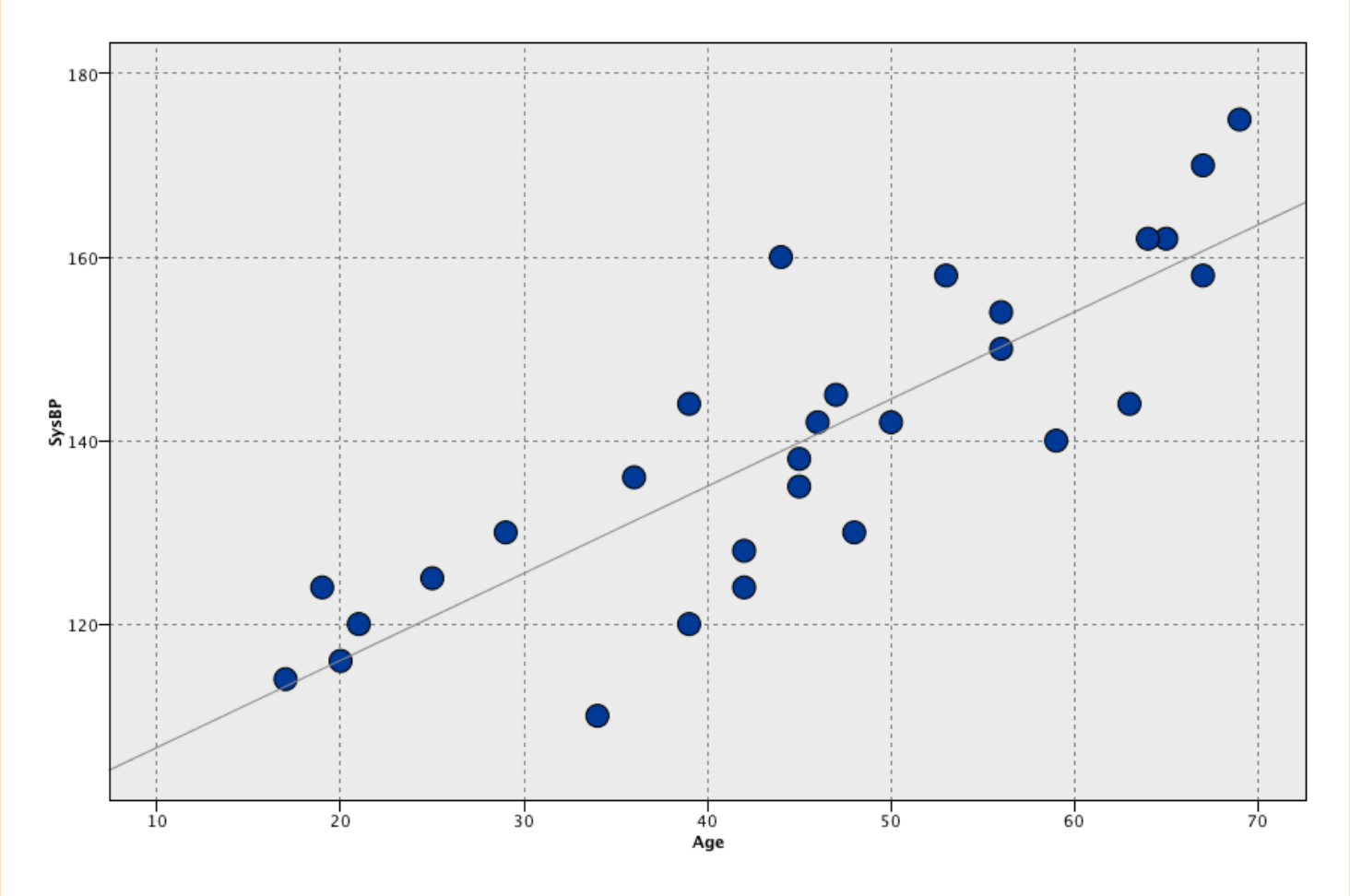


SysBP

Age

The real dataset with fitted line

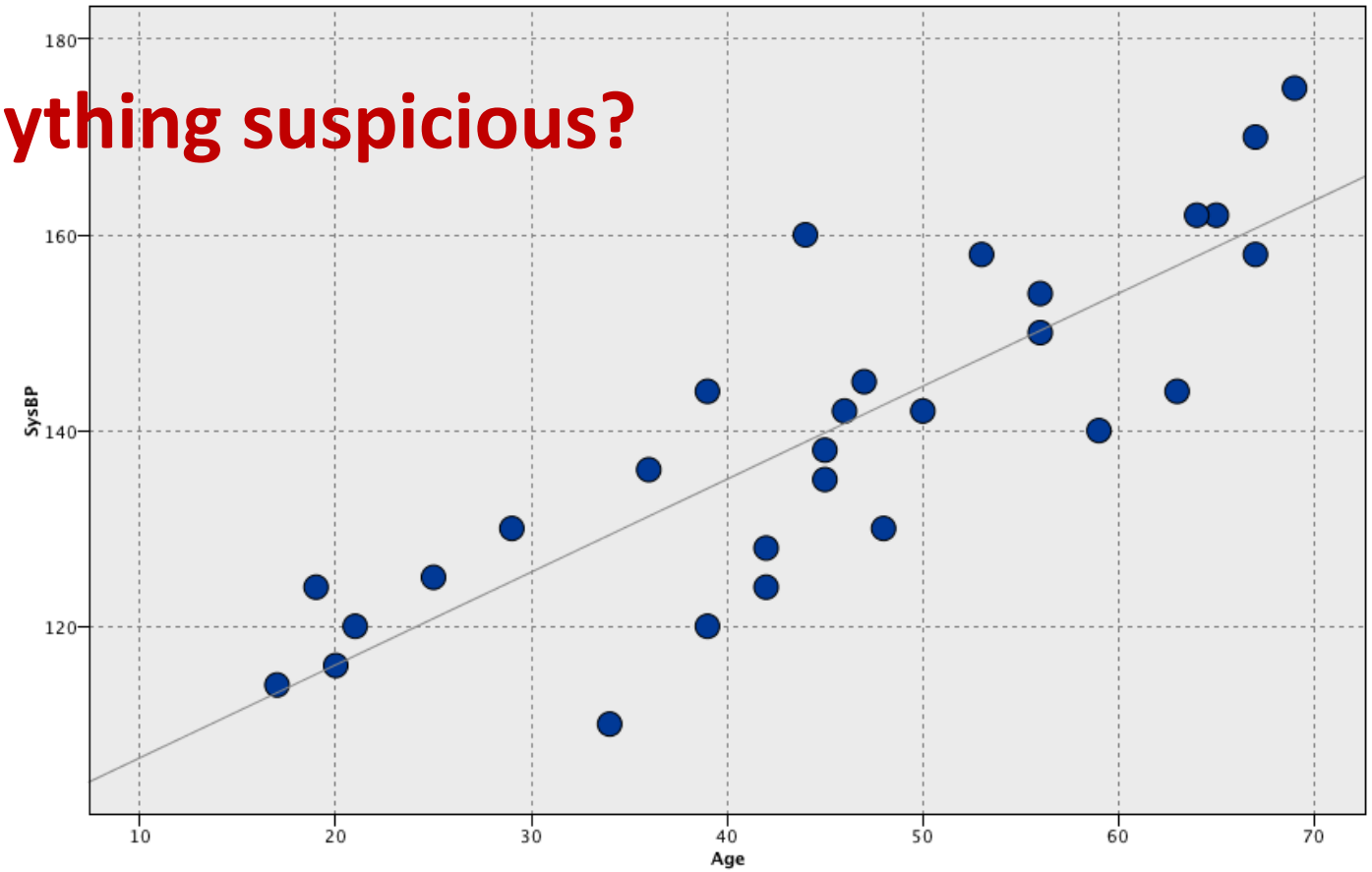
SysBP



Age

The real dataset

Anything suspicious?

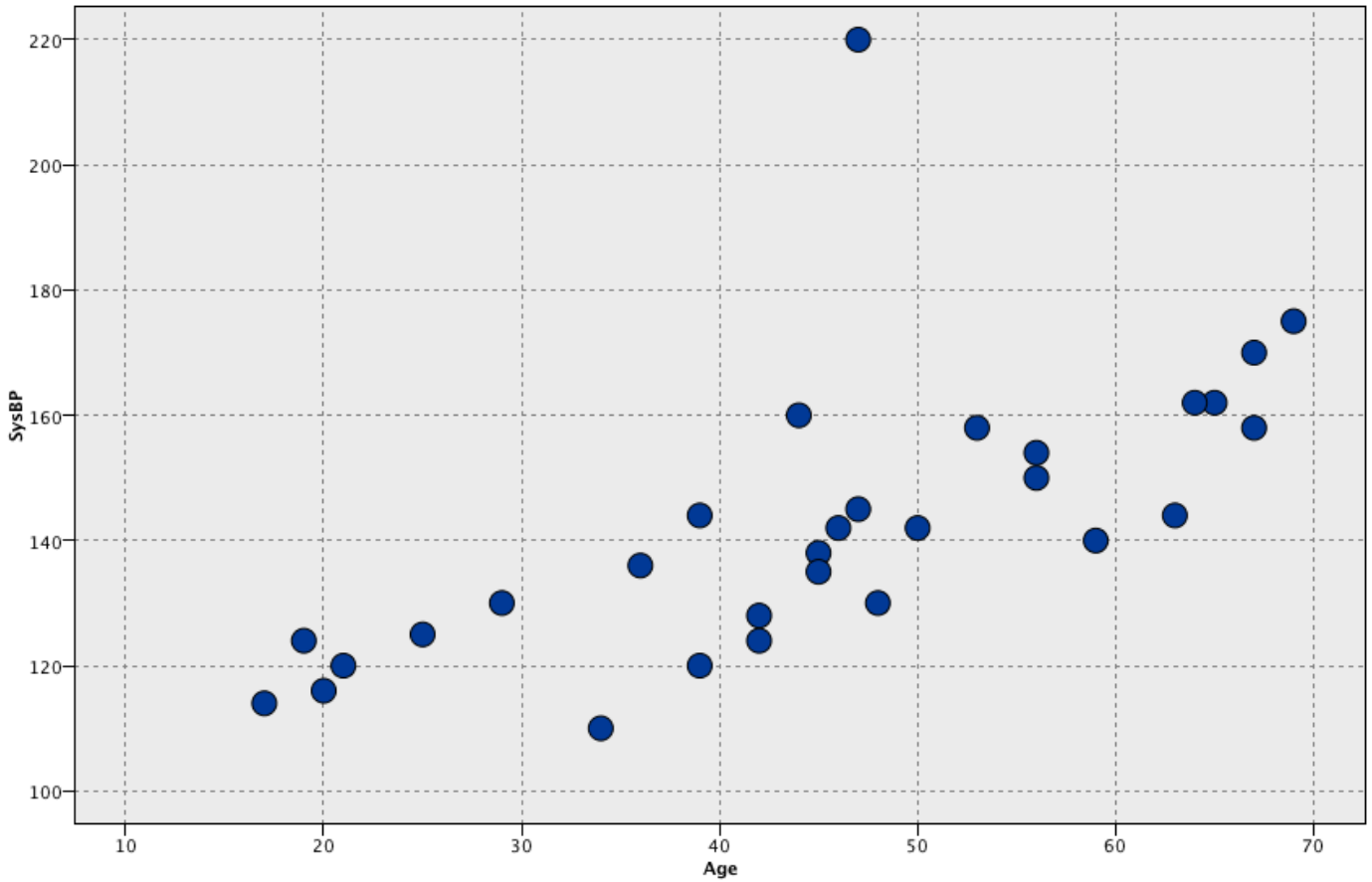


SysBP

Age

High blood pressure subject

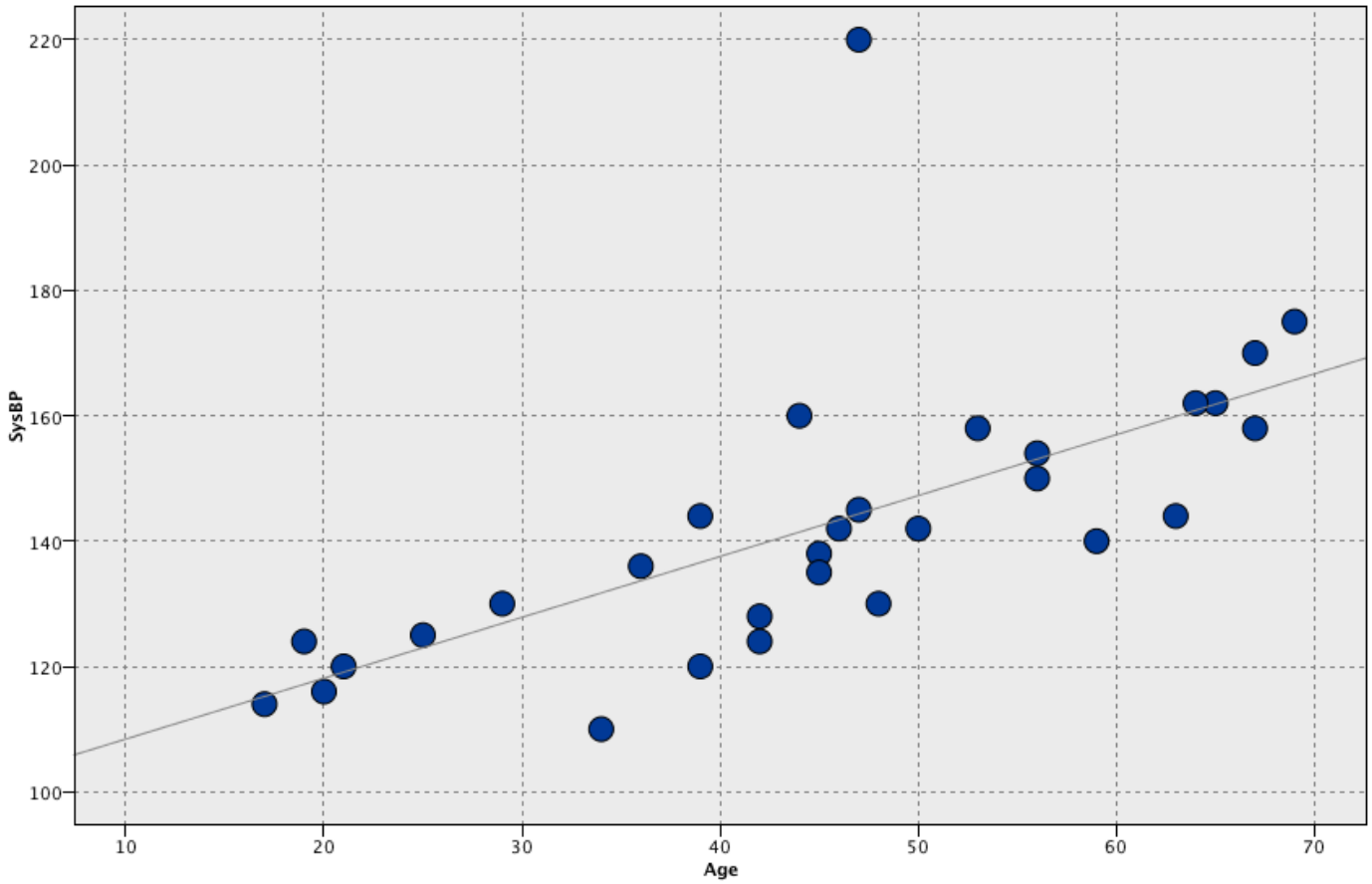
SysBP



Age

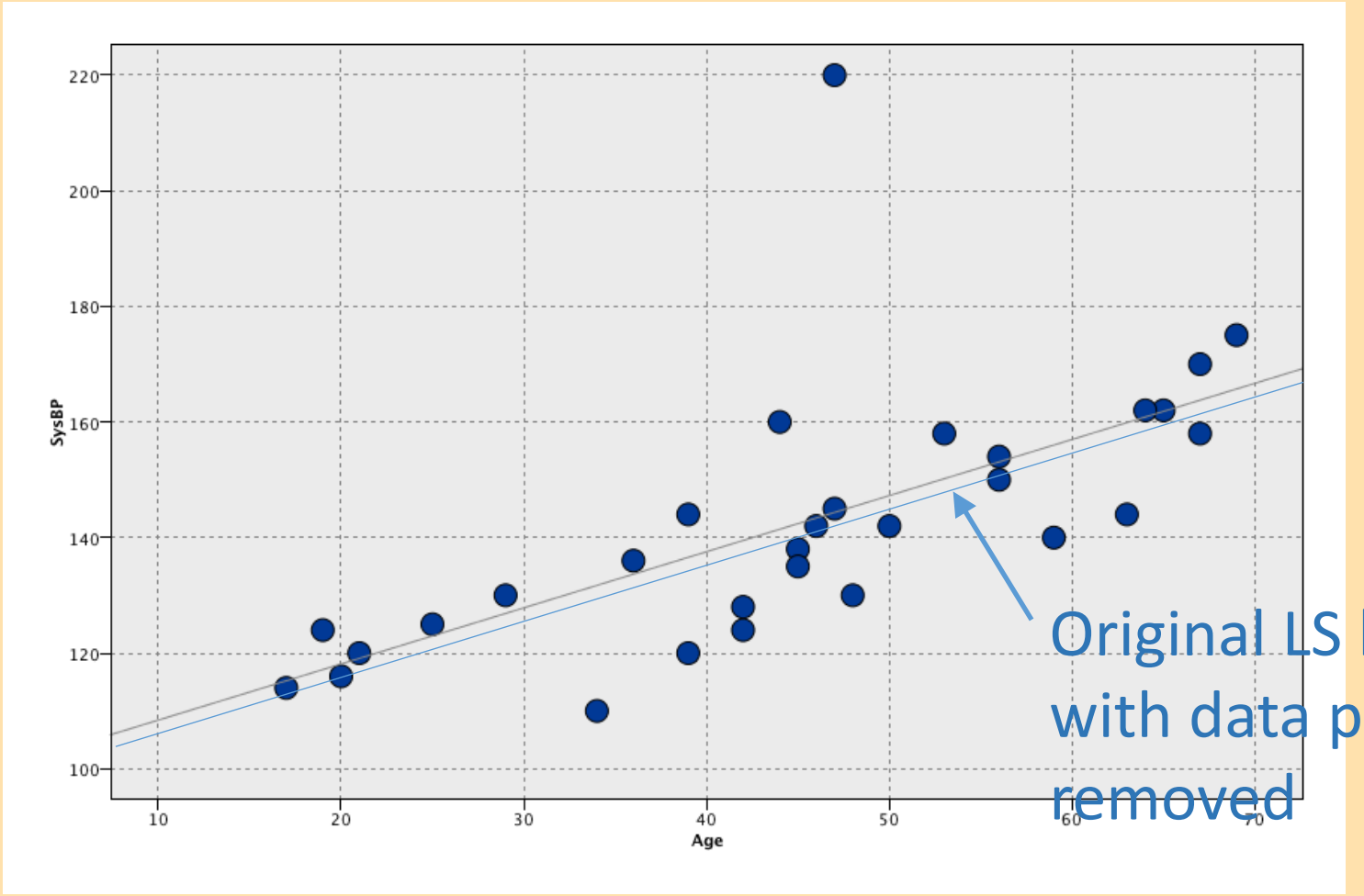
Fitted line

SysBP



Age

The real dataset

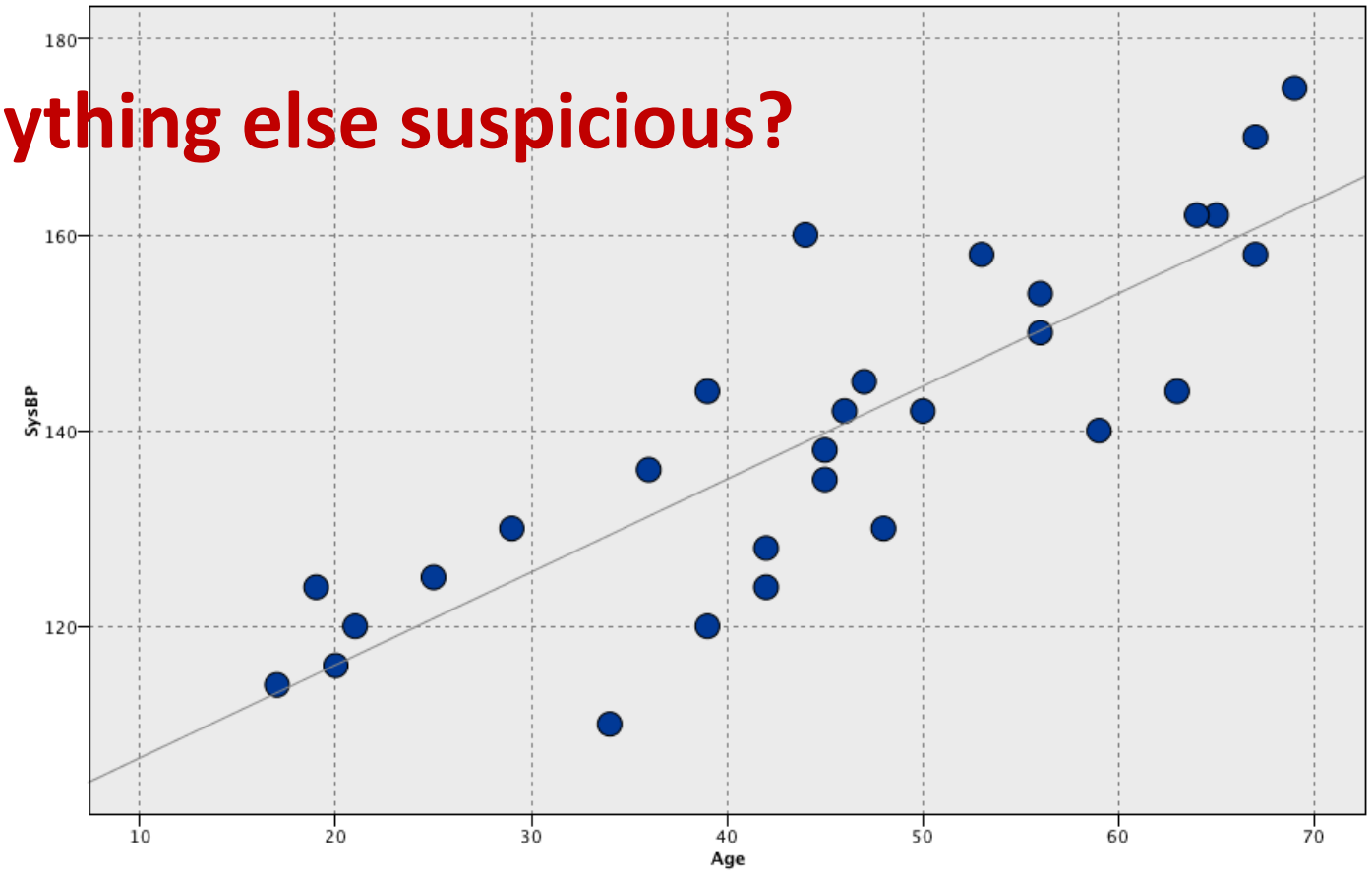


SysBP

Age

The real dataset

Anything else suspicious?



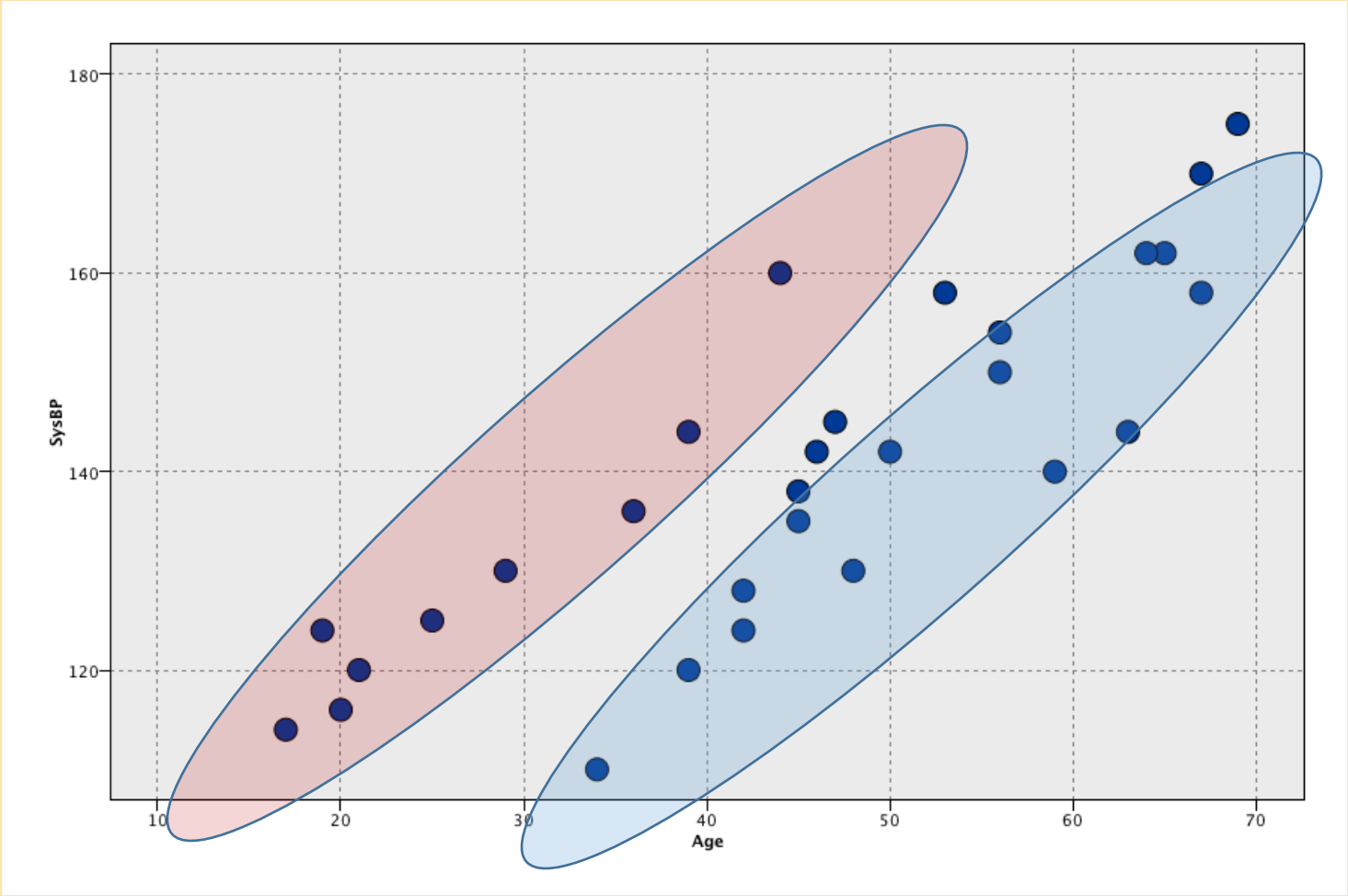
SysBP

Age

Is anything going on here?

Continuing with outlier dropped…

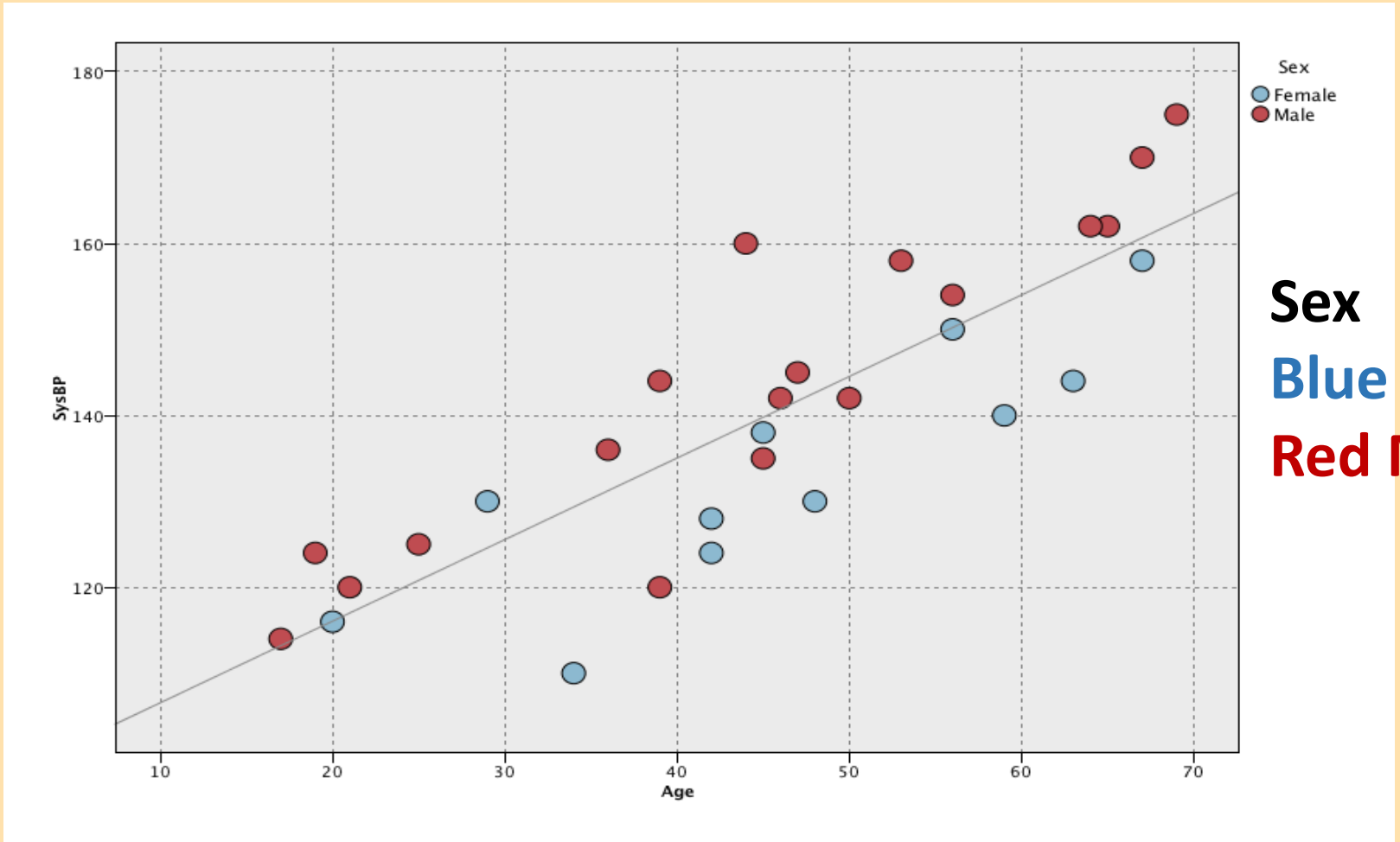
SysBP



Age

Separate by Sex

SysBP



Sex

Blue F

Red M

Age

Multi-predictor models

Now we might entertain a more complicated model:

$$y = ax + bz + c$$

e.g. y = Systolic BP (SysBP)

x = Age

z = Sex (1 = M, 0 = F)

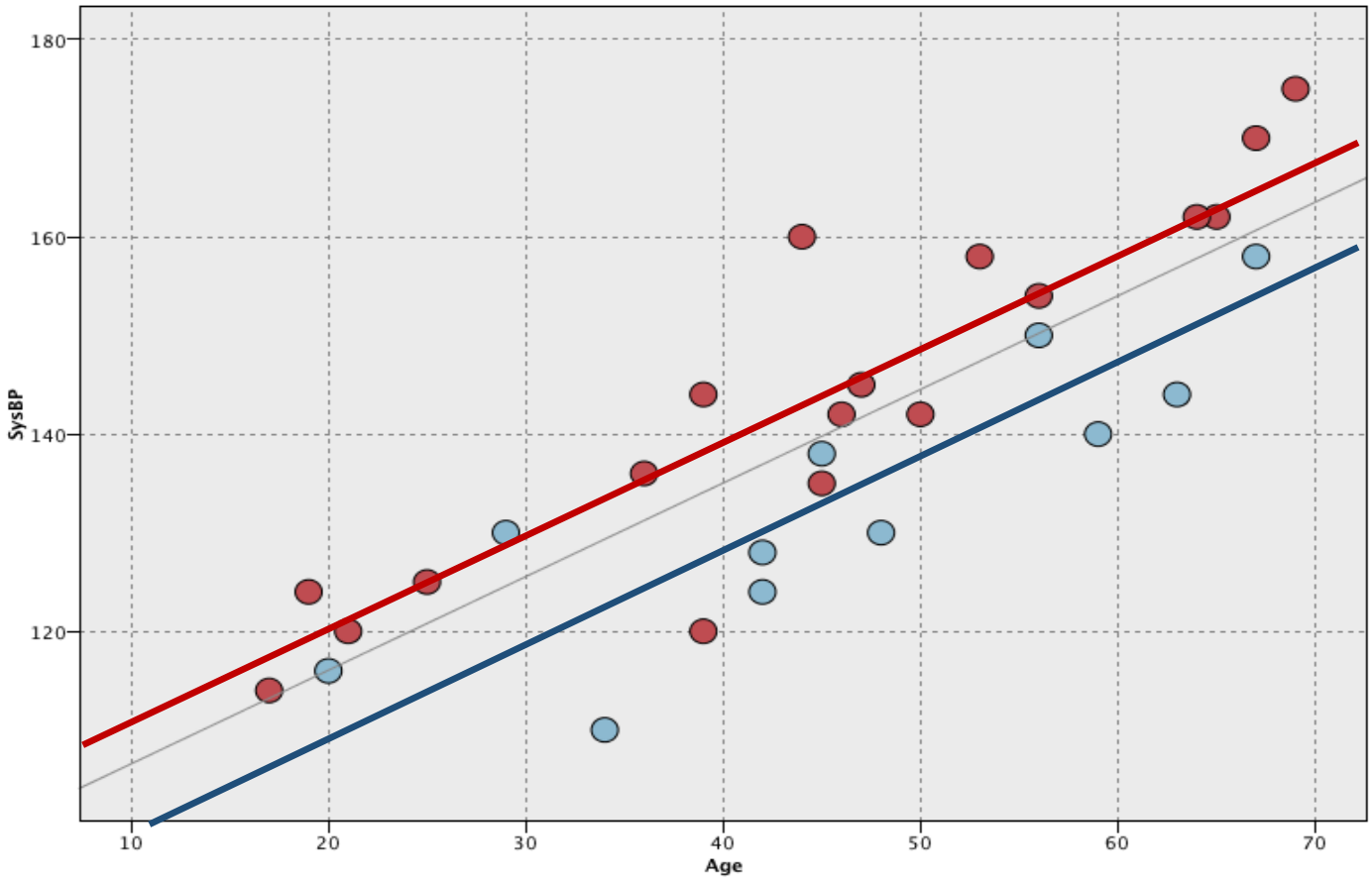
c = intercept (SysBP at age 0 and Sex = F)

a = change SysBP per year in Age

b = difference in SysBP for M vs. F

Question: Are Age and Sex predictive of SysBP?

Age *and* Sex as predictors



Sex

Blue F

Red M

Gray line = original fit, no sex predictor

SysBP

Age

And interactions

But why not even more complicated such as:

$$y = ax + bz + abw + c$$

e.g. y = Systolic BP (SysBP)

x = Age

z = Sex (1 = M, 0 = F)

c = intercept (SysBP at age 0 and Sex = F)

a = change in SysBP per year in Age for Sex = F

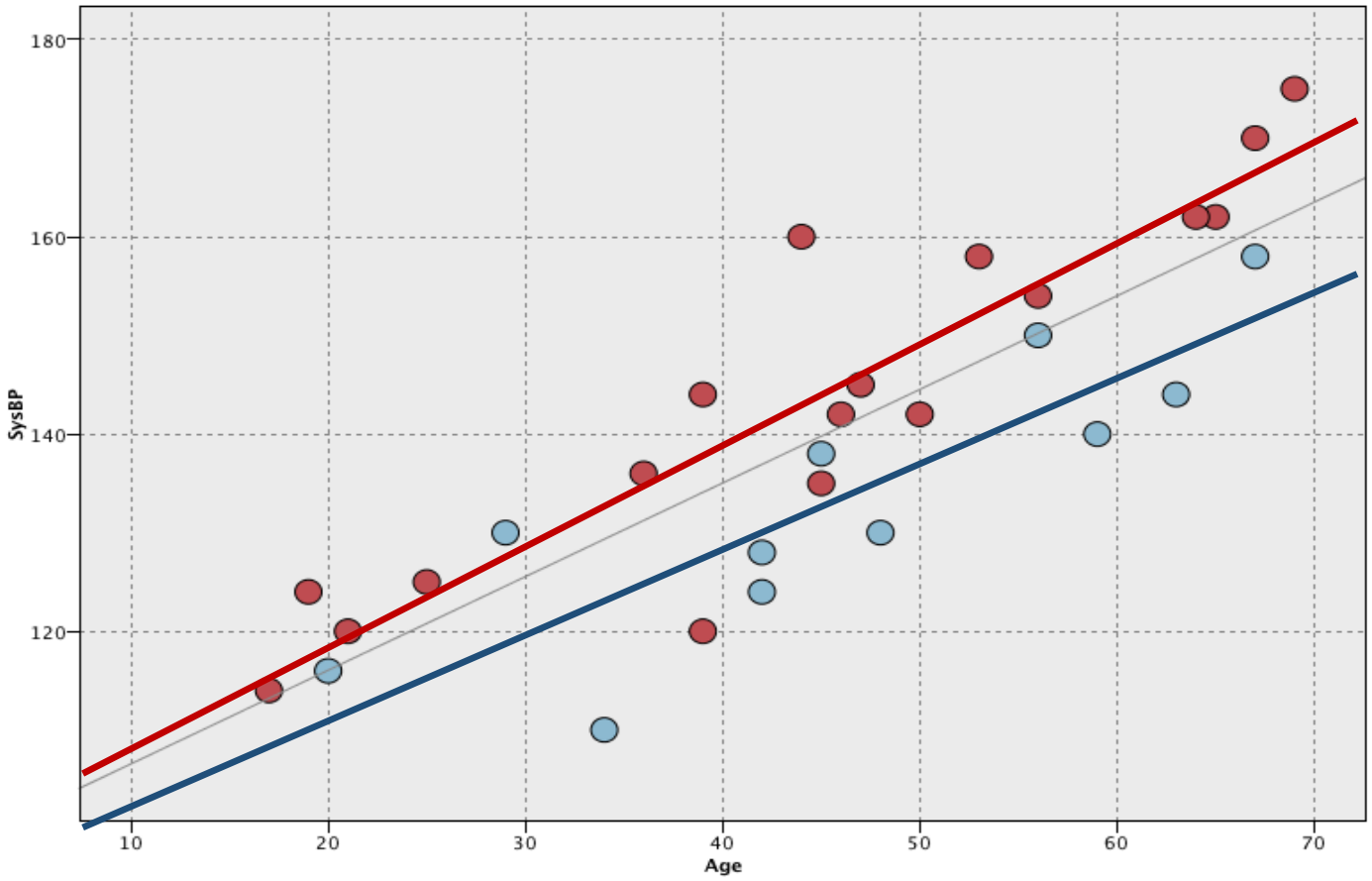
b = difference in SysBP for M vs. F at Age = 0

w = interaction effect - difference in SysBP per year in age for Sex = M vs. Sex = F

Question: Are Age and Sex and interaction of Age and Sex predictive of SysBP?

Age and Sex interaction

SysBP



Sex

Blue F

Red M

Gray line = original fit, no sex predictor

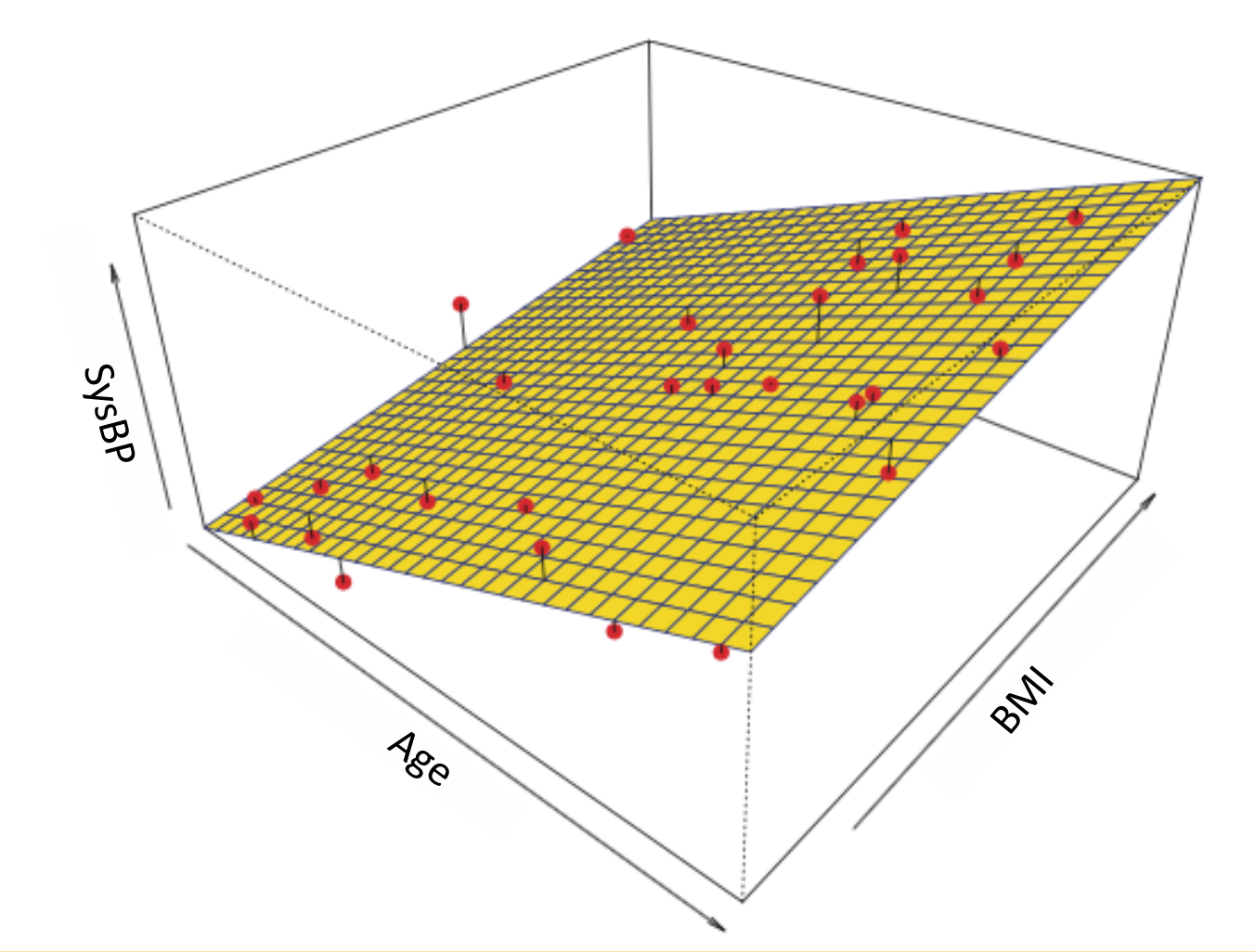
Age

Actually, no sex variable is in the dataset – I made it up for illustrative purposes

The doctored dataset is what is available on CLE in case you want to play with it…

Linear least squares with 2 (continuous) predictors

Adapted From ISLR



Many predictors

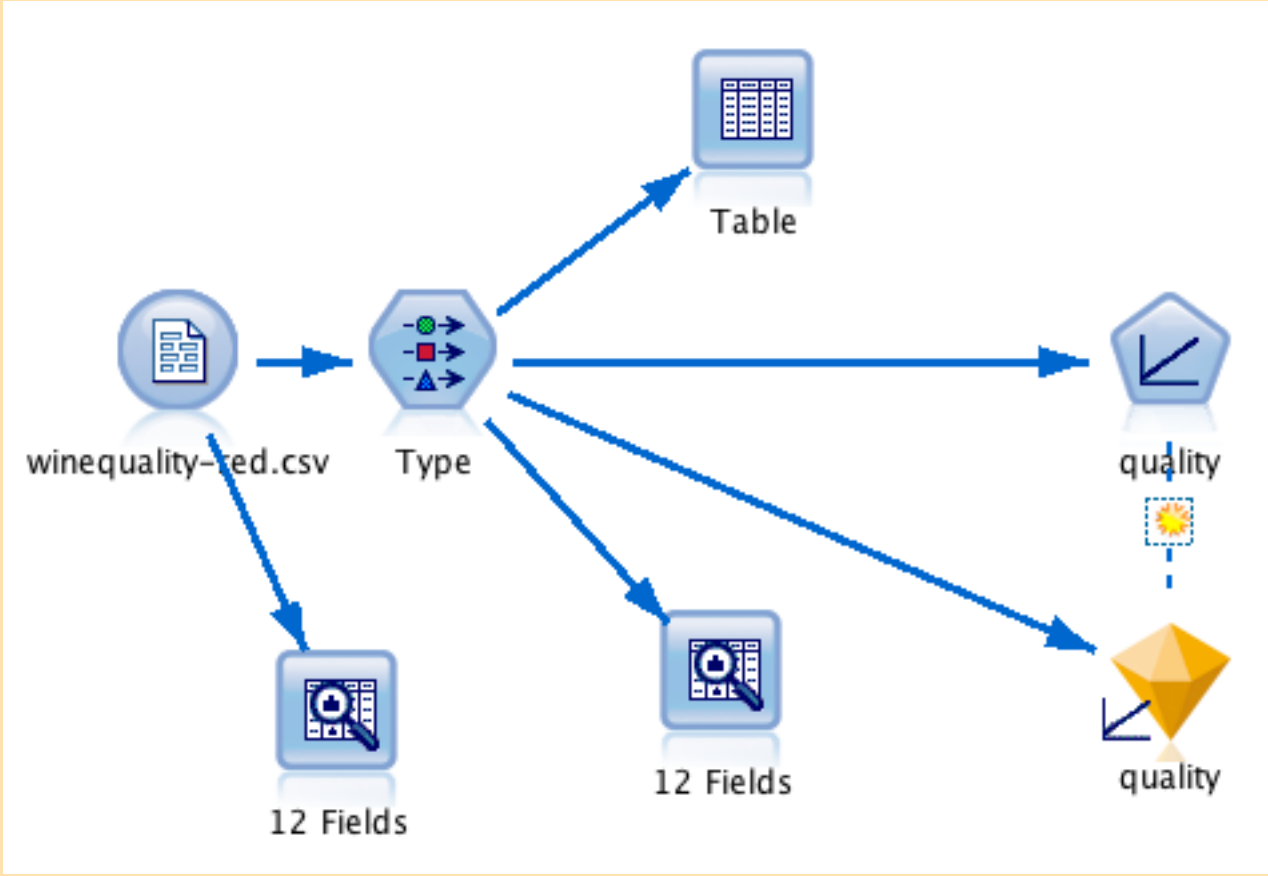
$$y = a_0 + a_1 x_1 + a_2 x_2 + \cdots + a_n x_n$$

- Fit n-dimensional hyper-plane in $(n+1)$-dimensional space
- The goal of some methods is to find a manageable subset of parameters that captures most of the predictive information – "variable selection methods" – Question of interest: Which of the variables $x_1, x_2, \ldots, x_n$ are predictive of y?
- Other methods don't worry about number of predictors explicitly, but rather just build a predictive "black box"

Wine dataset

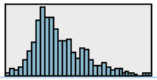
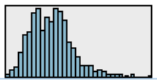
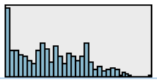
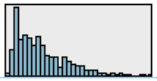
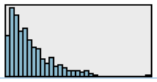
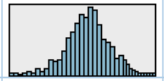
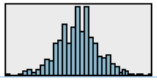
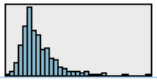
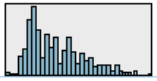
- *Wine Quality* dataset from UCI Machine Learning Repository https://archive.ics.uci.edu/ml/datasets.html (I also placed on CLE)
- Freely available dataset relating to Portuguese “Vinho Verde”
- P. Cortez, A. Cerdeira, F. Almeida, T. Matos and J. Reis. Modeling wine preferences by data mining from physicochemical properties. In Decision Support Systems, Elsevier, 47(4):547-553. ISSN: 0167-9236.
- Use objective test predictors (alcohol level, PH, acidity, etc.) to predict wine expert subjective assessments: median of 3 experts scoring 0 (very bad) to 10 (very excellent)
- No missing attributes
- We will focus on the “red variant” dataset (on CLE)

Multiple Regression Stream



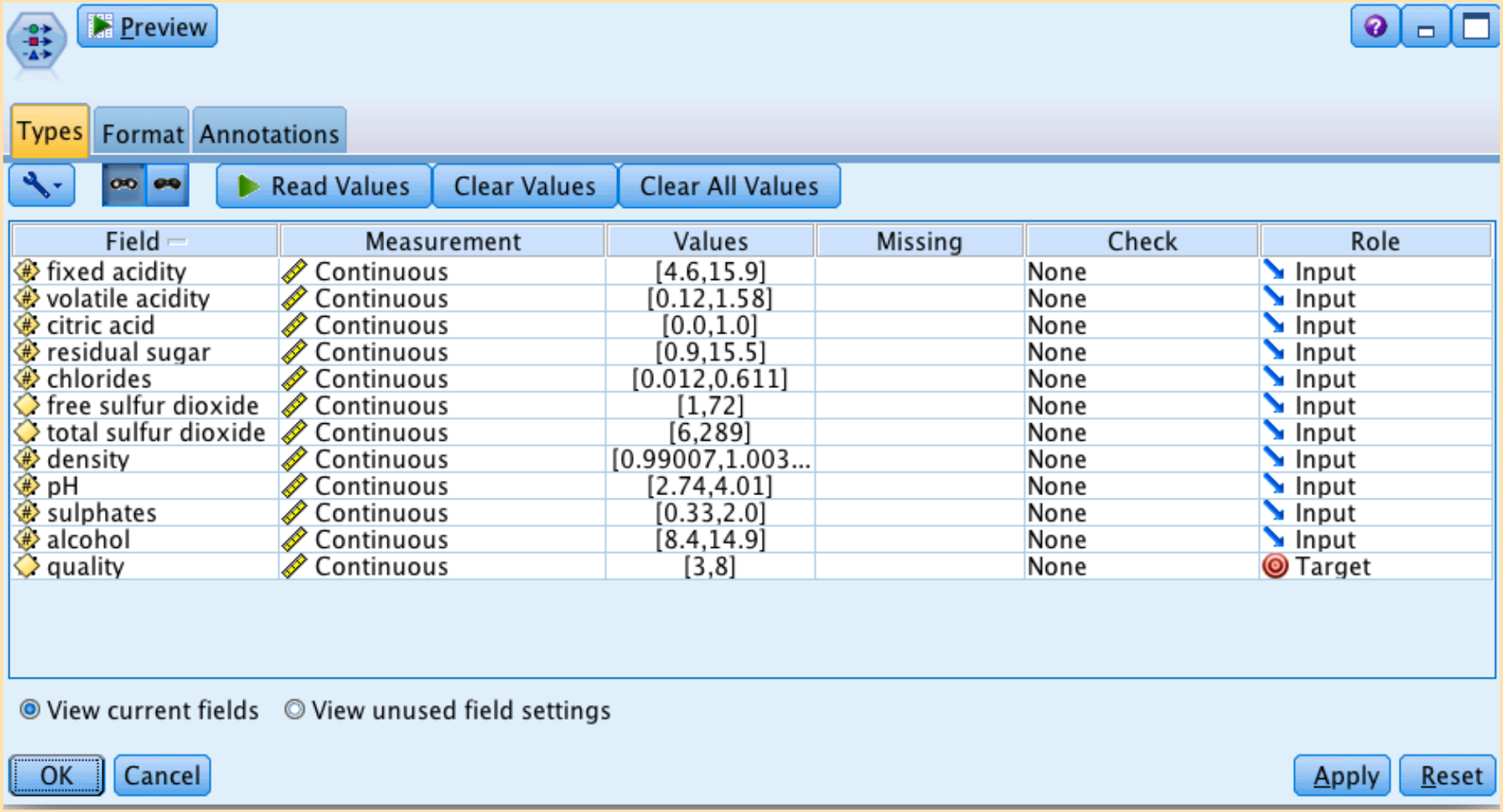
Data Audit prior to Type

Audit | Quality | Annotations

Field	Graph	Measurement	Min	Max	Mean	Std. Dev	Skewness	Unique	Valid
fixed acidity		Continuous	4.600	15.900	8.320	1.741	0.983	--	1599
volatile acidity		Continuous	0.120	1.580	0.528	0.179	0.672	--	1599
citric acid		Continuous	0.000	1.000	0.271	0.195	0.318	--	1599
residual sugar		Continuous	0.900	15.500	2.539	1.410	4.541	--	1599
chlorides		Continuous	0.012	0.611	0.087	0.047	5.680	--	1599
free sulfur dioxi...		Continuous	1	72	15.874	10.458	1.250	--	1599
total sulfur diox...		Continuous	6	289	46.467	32.895	1.516	--	1599
density		Continuous	0.990	1.004	0.997	0.002	0.071	--	1599
pH		Continuous	2.740	4.010	3.311	0.154	0.194	--	1599
sulphates		Continuous	0.330	2.000	0.658	0.170	2.429	--	1599
alcohol		Continuous	8.400	14.900	10.423	1.066	0.861	--	1599
quality		Continuous	3	8	5.636	0.808	0.218	--	1599

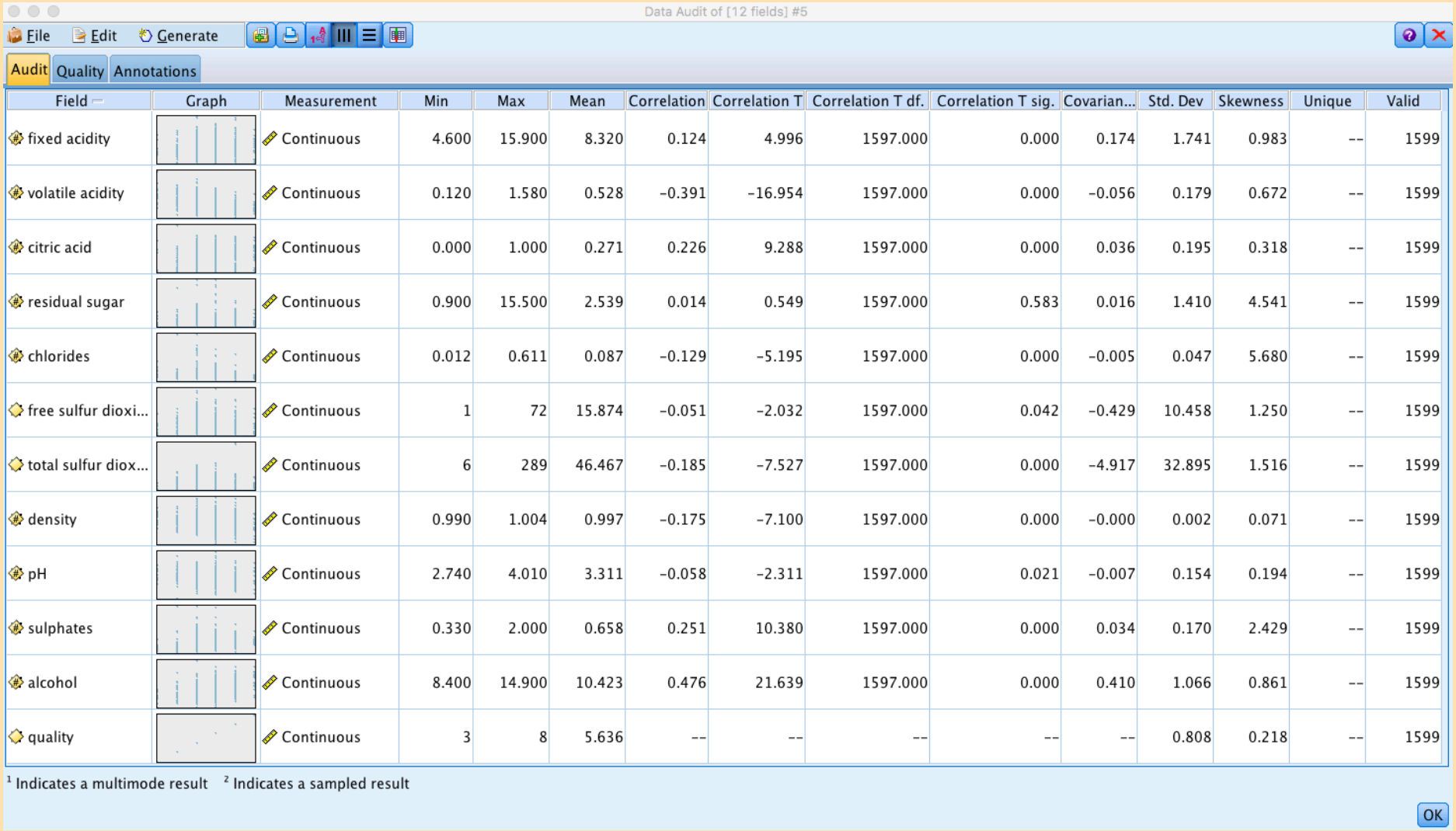
[1] Indicates a multimode result [2] Indicates a sampled result

Type Node



Field	Measurement	Values	Missing	Check	Role
fixed acidity	Continuous	[4.6,15.9]		None	Input
volatile acidity	Continuous	[0.12,1.58]		None	Input
citric acid	Continuous	[0.0,1.0]		None	Input
residual sugar	Continuous	[0.9,15.5]		None	Input
chlorides	Continuous	[0.012,0.611]		None	Input
free sulfur dioxide	Continuous	[1,72]		None	Input
total sulfur dioxide	Continuous	[6,289]		None	Input
density	Continuous	[0.99007,1.003...		None	Input
pH	Continuous	[2.74,4.01]		None	Input
sulphates	Continuous	[0.33,2.0]		None	Input
alcohol	Continuous	[8.4,14.9]		None	Input
quality	Continuous	[3,8]		None	Target

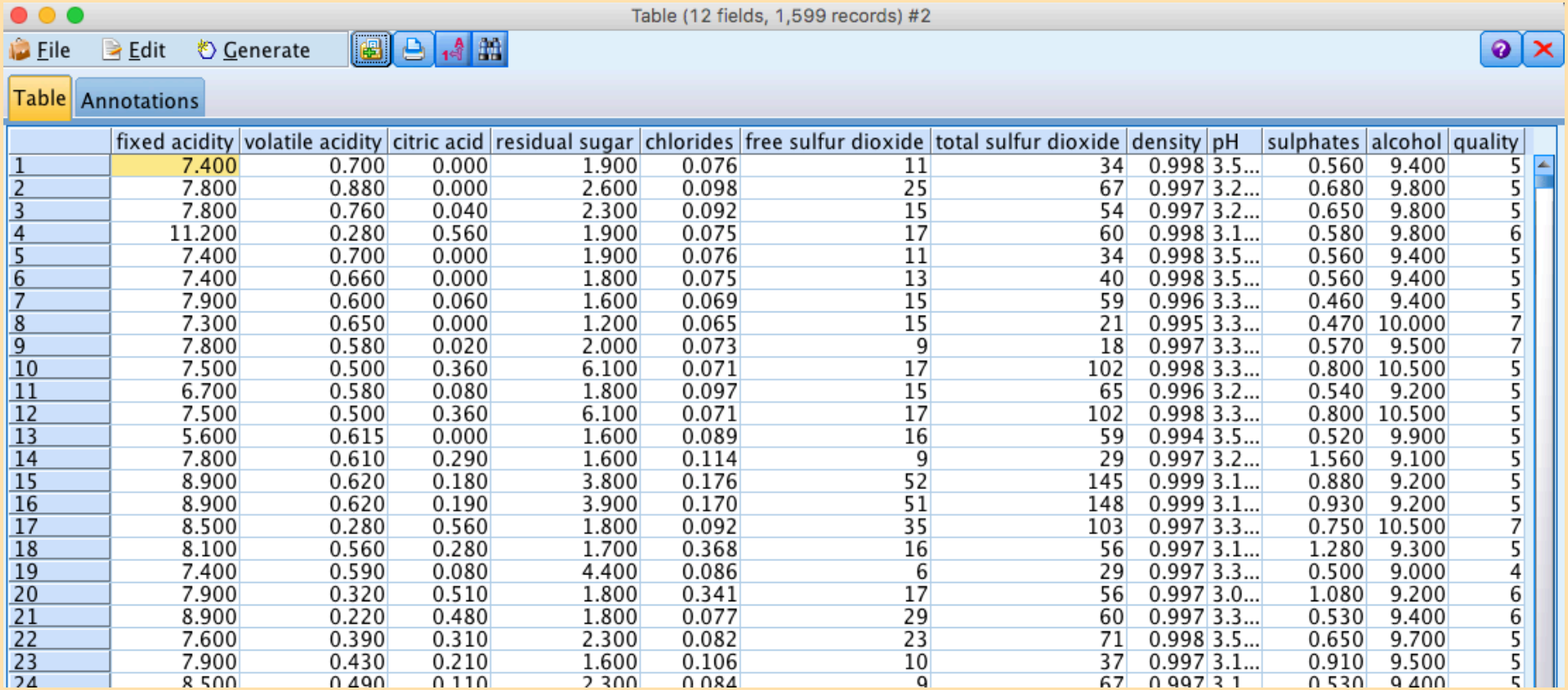
Data Audit post Type



Field	Graph	Measurement	Min	Max	Mean	Correlation	Correlation T	Correlation T df.	Correlation T sig.	Covarian...	Std. Dev	Skewness	Unique	Valid
fixed acidity		Continuous	4.600	15.900	8.320	0.124	4.996	1597.000	0.000	0.174	1.741	0.983	--	1599
volatile acidity		Continuous	0.120	1.580	0.528	-0.391	-16.954	1597.000	0.000	-0.056	0.179	0.672	--	1599
citric acid		Continuous	0.000	1.000	0.271	0.226	9.288	1597.000	0.000	0.036	0.195	0.318	--	1599
residual sugar		Continuous	0.900	15.500	2.539	0.014	0.549	1597.000	0.583	0.016	1.410	4.541	--	1599
chlorides		Continuous	0.012	0.611	0.087	-0.129	-5.195	1597.000	0.000	-0.005	0.047	5.680	--	1599
free sulfur dioxi...		Continuous	1	72	15.874	-0.051	-2.032	1597.000	0.042	-0.429	10.458	1.250	--	1599
total sulfur diox...		Continuous	6	289	46.467	-0.185	-7.527	1597.000	0.000	-4.917	32.895	1.516	--	1599
density		Continuous	0.990	1.004	0.997	-0.175	-7.100	1597.000	0.000	-0.000	0.002	0.071	--	1599
pH		Continuous	2.740	4.010	3.311	-0.058	-2.311	1597.000	0.021	-0.007	0.154	0.194	--	1599
sulphates		Continuous	0.330	2.000	0.658	0.251	10.380	1597.000	0.000	0.034	0.170	2.429	--	1599
alcohol		Continuous	8.400	14.900	10.423	0.476	21.639	1597.000	0.000	0.410	1.066	0.861	--	1599
quality		Continuous	3	8	5.636	--	--	--	--	--	0.808	0.218	--	1599

[1] Indicates a multimode result [2] Indicates a sampled result

Output of Table node

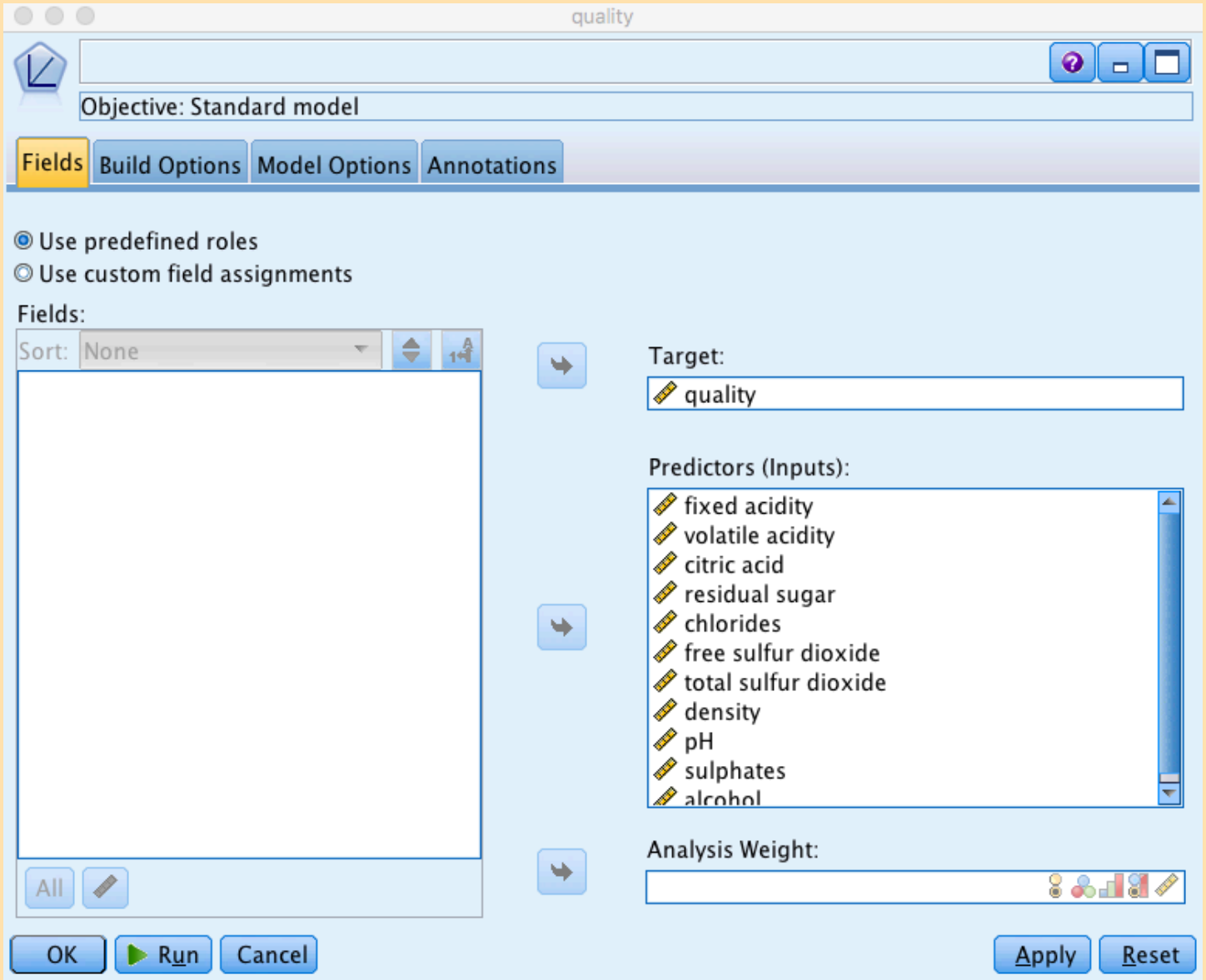


	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates	alcohol	quality
1	7.400	0.700	0.000	1.900	0.076	11	34	0.998	3.5...	0.560	9.400	5
2	7.800	0.880	0.000	2.600	0.098	25	67	0.997	3.2...	0.680	9.800	5
3	7.800	0.760	0.040	2.300	0.092	15	54	0.997	3.2...	0.650	9.800	5
4	11.200	0.280	0.560	1.900	0.075	17	60	0.998	3.1...	0.580	9.800	6
5	7.400	0.700	0.000	1.900	0.076	11	34	0.998	3.5...	0.560	9.400	5
6	7.400	0.660	0.000	1.800	0.075	13	40	0.998	3.5...	0.560	9.400	5
7	7.900	0.600	0.060	1.600	0.069	15	59	0.996	3.3...	0.460	9.400	5
8	7.300	0.650	0.000	1.200	0.065	15	21	0.995	3.3...	0.470	10.000	7
9	7.800	0.580	0.020	2.000	0.073	9	18	0.997	3.3...	0.570	9.500	7
10	7.500	0.500	0.360	6.100	0.071	17	102	0.998	3.3...	0.800	10.500	5
11	6.700	0.580	0.080	1.800	0.097	15	65	0.996	3.2...	0.540	9.200	5
12	7.500	0.500	0.360	6.100	0.071	17	102	0.998	3.3...	0.800	10.500	5
13	5.600	0.615	0.000	1.600	0.089	16	59	0.994	3.5...	0.520	9.900	5
14	7.800	0.610	0.290	1.600	0.114	9	29	0.997	3.2...	1.560	9.100	5
15	8.900	0.620	0.180	3.800	0.176	52	145	0.999	3.1...	0.880	9.200	5
16	8.900	0.620	0.190	3.900	0.170	51	148	0.999	3.1...	0.930	9.200	5
17	8.500	0.280	0.560	1.800	0.092	35	103	0.997	3.3...	0.750	10.500	7
18	8.100	0.560	0.280	1.700	0.368	16	56	0.997	3.1...	1.280	9.300	5
19	7.400	0.590	0.080	4.400	0.086	6	29	0.997	3.3...	0.500	9.000	4
20	7.900	0.320	0.510	1.800	0.341	17	56	0.997	3.0...	1.080	9.200	6
21	8.900	0.220	0.480	1.800	0.077	29	60	0.997	3.3...	0.530	9.400	6
22	7.600	0.390	0.310	2.300	0.082	23	71	0.998	3.5...	0.650	9.700	5
23	7.900	0.430	0.210	1.600	0.106	10	37	0.997	3.1...	0.910	9.500	5
24	8.500	0.490	0.110	2.300	0.084	9	67	0.997	3.1	0.530	9.400	5

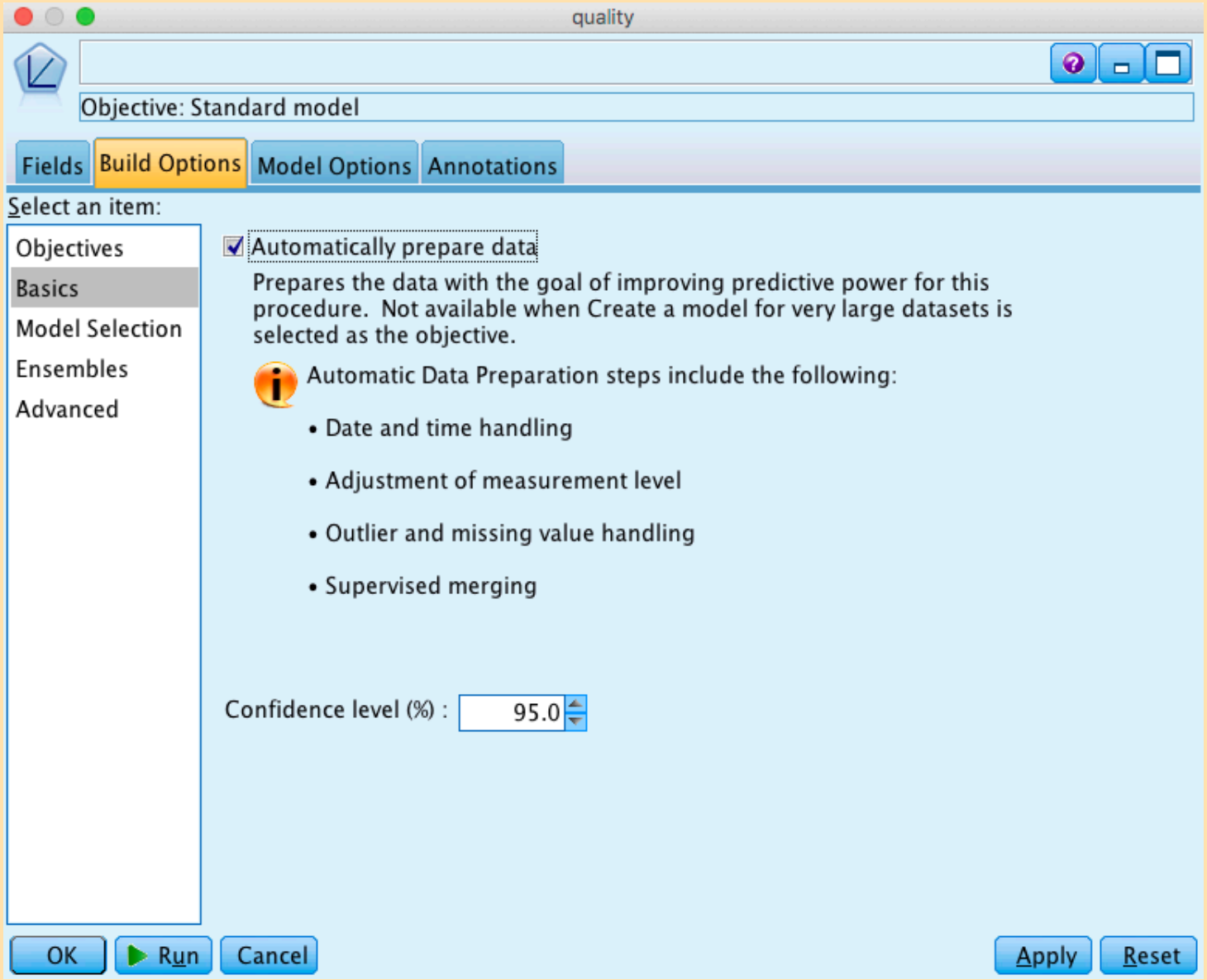
. . .

. . .

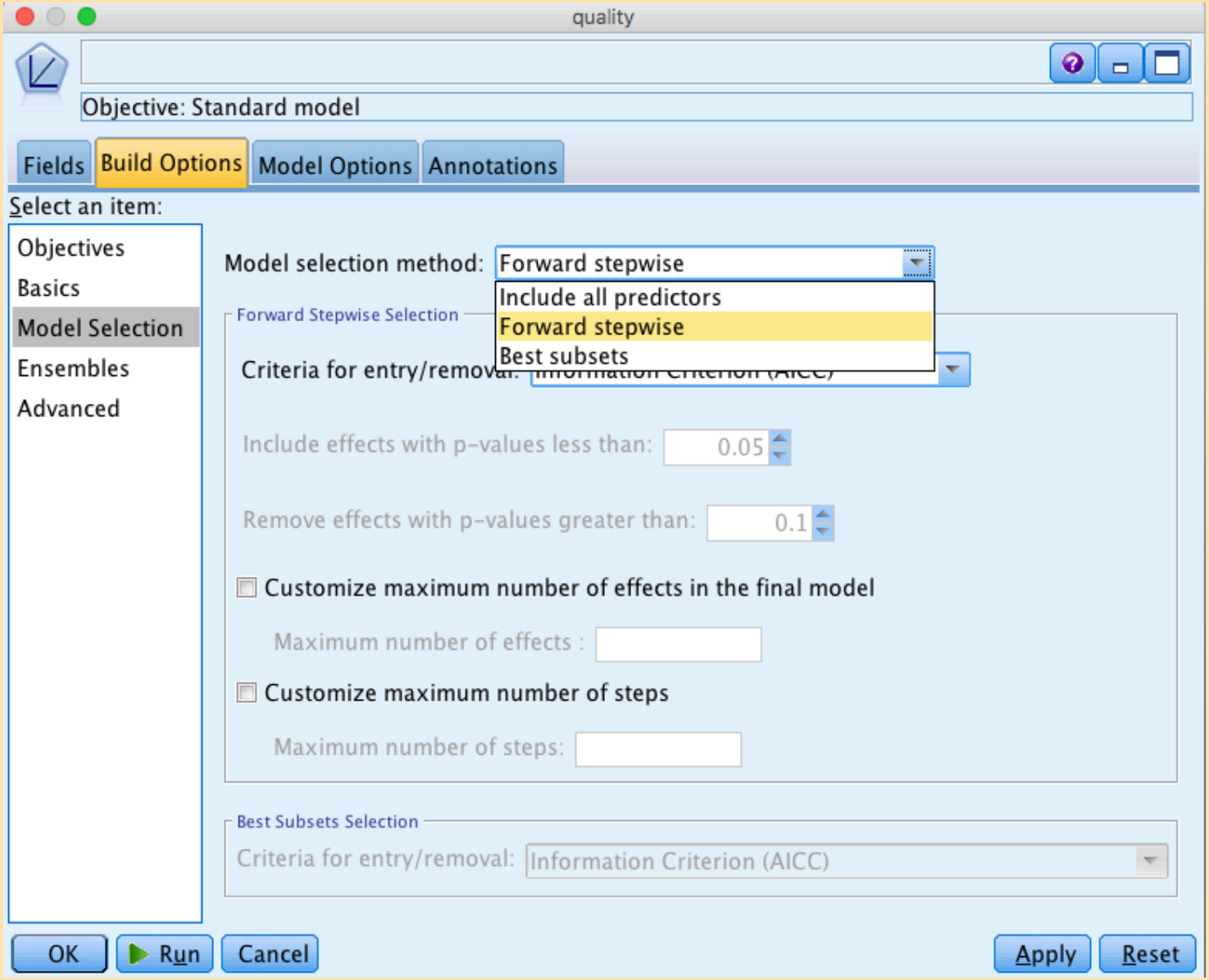
Linear node


quality
Objective: Standard model
Fields
Build Options
Model Options
Annotations
Use predefined roles
Use custom field assignments
Fields:
Sort:
None
All
Target:
quality
Predictors (Inputs):
fixed acidity
volatile acidity
citric acid
residual sugar
chlorides
free sulfur dioxide
total sulfur dioxide
density
pH
sulphates
alcohol
Analysis Weight:
OK
Run
Cancel
Apply
Reset

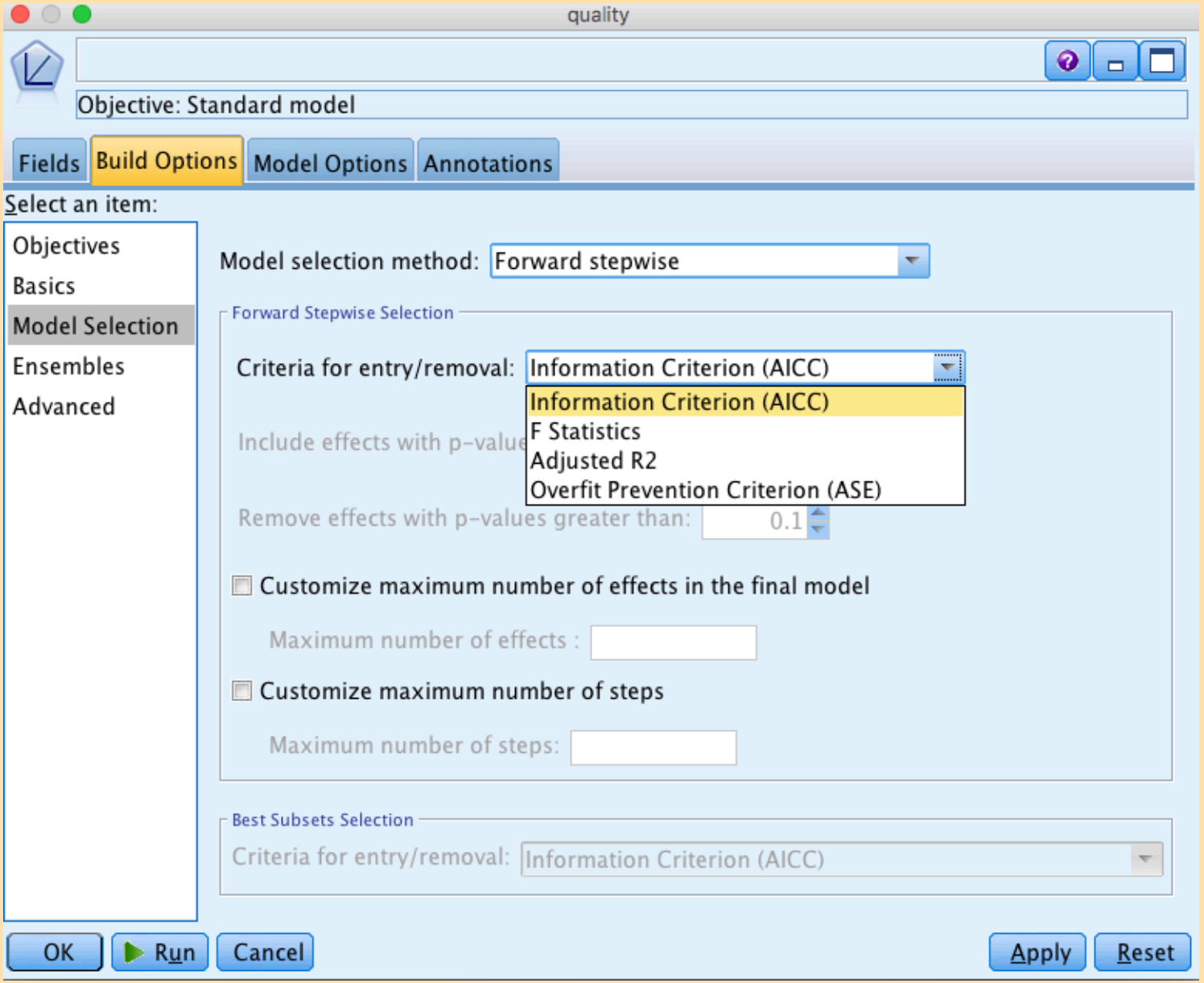
Linear node


quality
Objective: Standard model
Fields
Build Options
Model Options
Annotations
Select an item:
Objectives
Basics
Model Selection
Ensembles
Advanced
Automatically prepare data
Prepares the data with the goal of improving predictive power for this procedure. Not available when Create a model for very large datasets is selected as the objective.
Automatic Data Preparation steps include the following:
• Date and time handling
• Adjustment of measurement level
• Outlier and missing value handling
• Supervised merging
Confidence level (%) :
95.0
OK
Run
Cancel
Apply
Reset

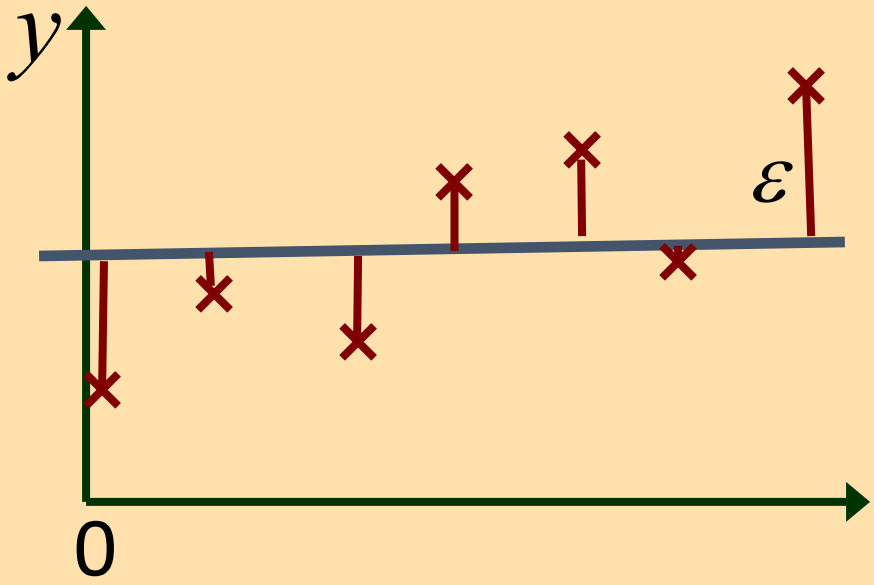
Linear node


quality
Objective: Standard model
Fields
Build Options
Model Options
Annotations
Select an item:
Objectives
Basics
Model Selection
Ensembles
Advanced
Model selection method:
Forward stepwise
Include all predictors
Forward stepwise
Best subsets
Forward Stepwise Selection
Criteria for entry/removal:
Include effects with p-values less than:
0.05
Remove effects with p-values greater than:
0.1
Customize maximum number of effects in the final model
Maximum number of effects :
Customize maximum number of steps
Maximum number of steps:
Best Subsets Selection
Criteria for entry/removal:
Information Criterion (AICC)
OK
Run
Cancel
Apply
Reset

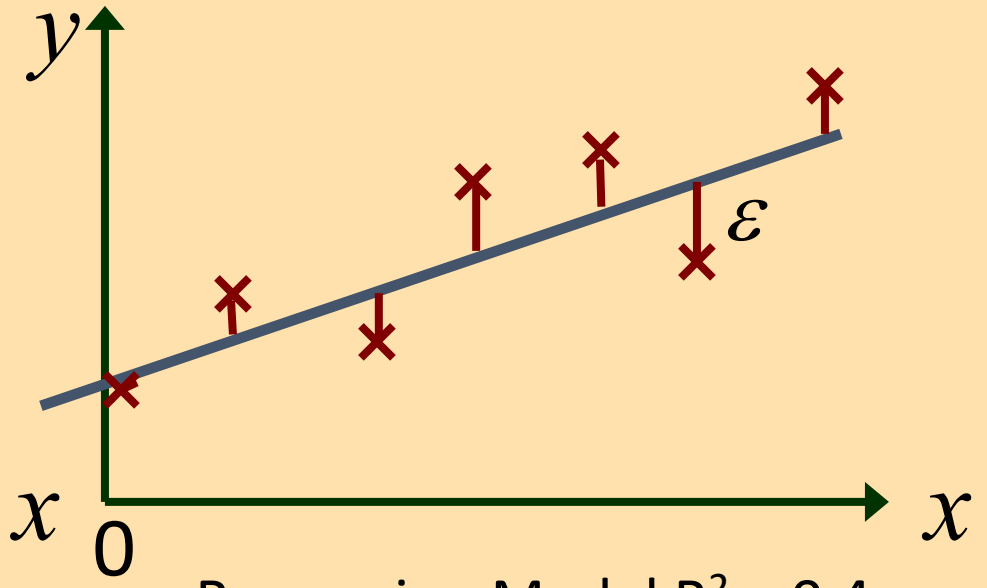
Linear node


quality
Objective: Standard model
Fields
Build Options
Model Options
Annotations
Select an item:
Objectives
Basics
Model Selection
Ensembles
Advanced
Model selection method:
Forward stepwise
Forward Stepwise Selection
Criteria for entry/removal:
Information Criterion (AICC)
Information Criterion (AICC)
F Statistics
Adjusted R2
Overfit Prevention Criterion (ASE)
Include effects with p-value
Remove effects with p-values greater than:
0.1
Customize maximum number of effects in the final model
Maximum number of effects :
Customize maximum number of steps
Maximum number of steps:
Best Subsets Selection
Criteria for entry/removal:
Information Criterion (AICC)
OK
Run
Cancel
Apply
Reset

R^2



Null Model $R^2 = 0$

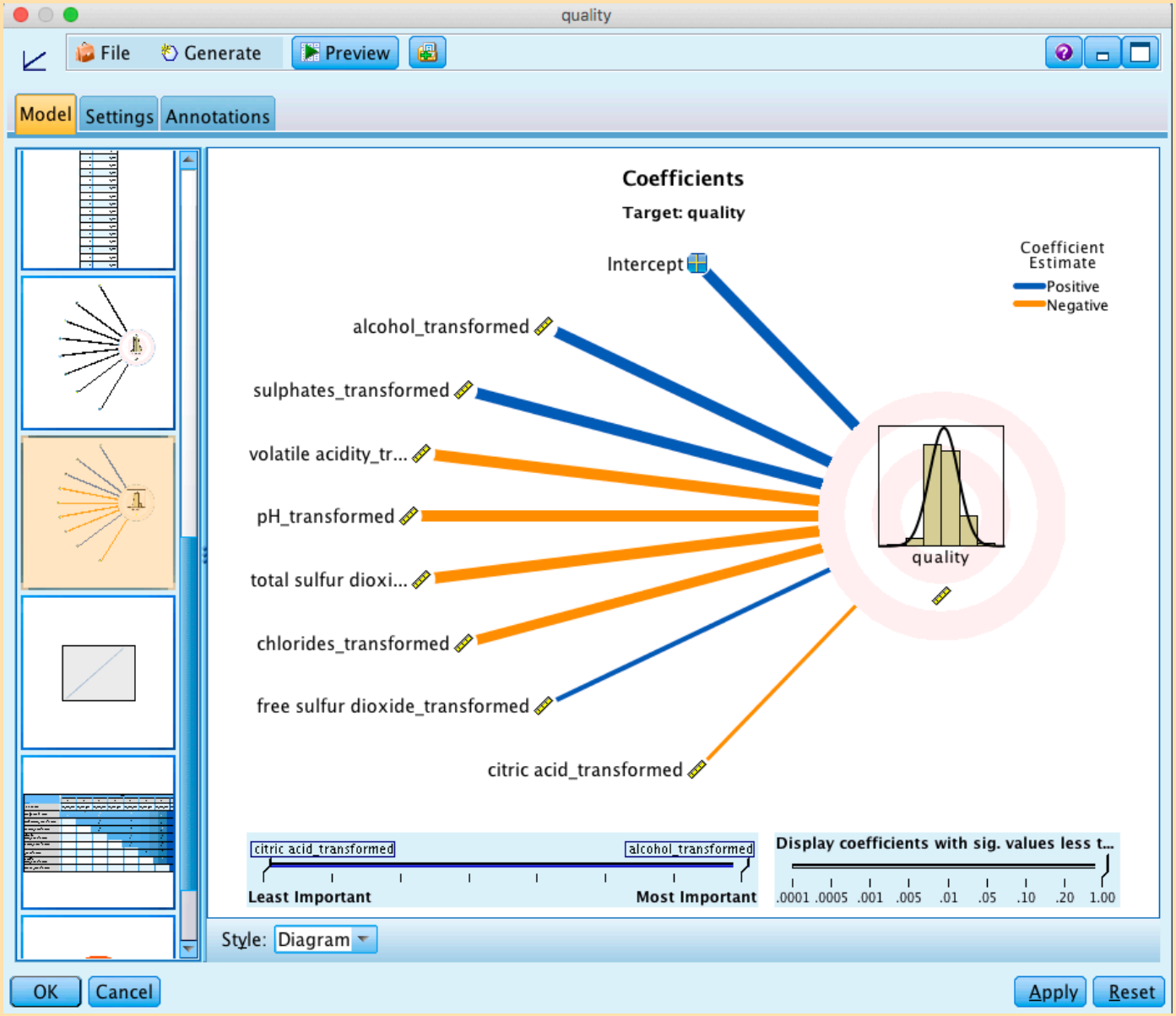


Regression Model $R^2 = 0.4$
40% of variance is explained by regression line

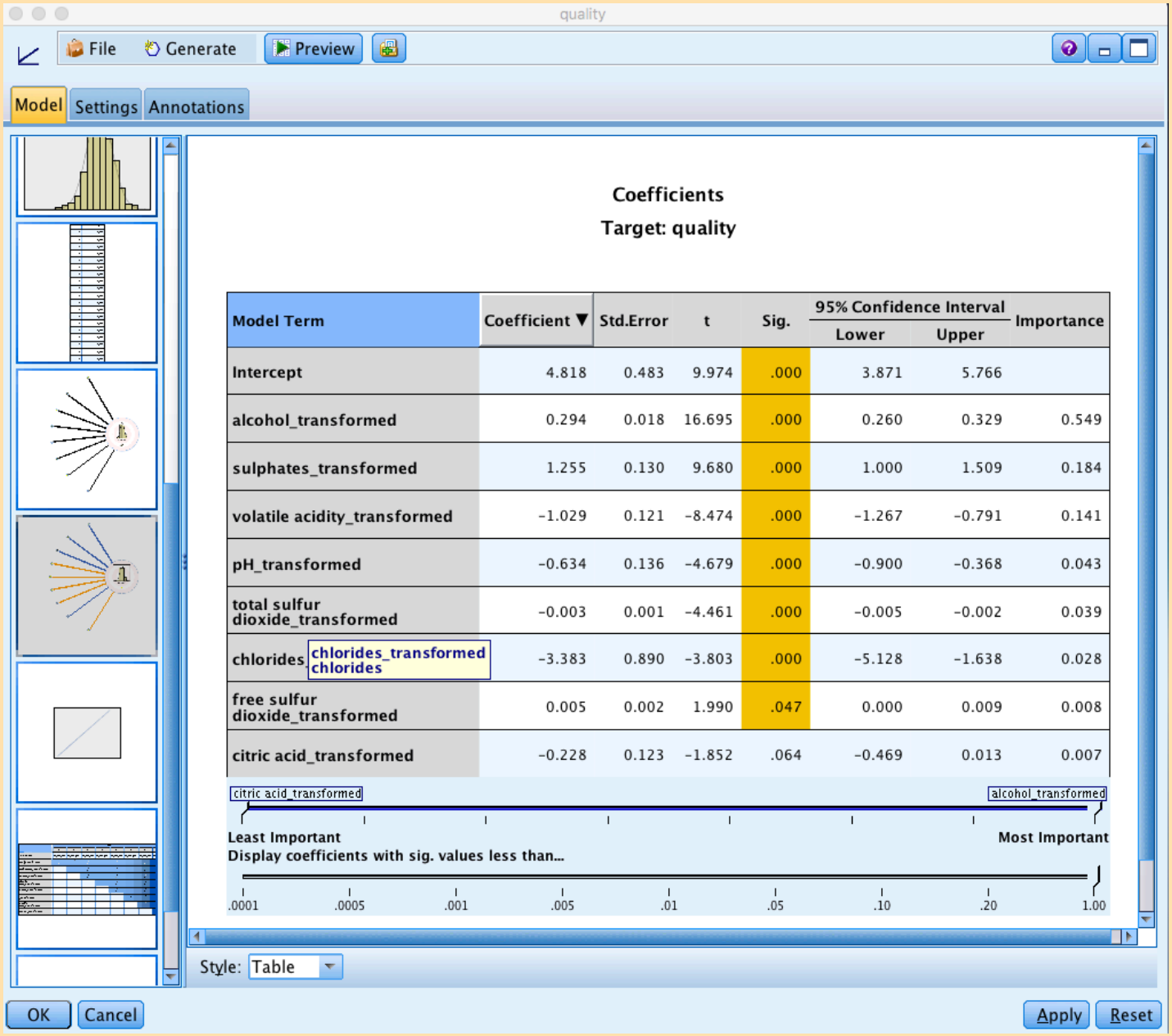
$$R^2 = 1 - {SS_{model}}/{SS_{null}}$$

Adjusted R^2 also adjusts for the number of predictors/model complexity

Golden Nugget



Coefficients



Model Term	Coefficient ▼	Std.Error	t	Sig.	95% Confidence Interval		Importance
					Lower	Upper	
Intercept	4.818	0.483	9.974	.000	3.871	5.766	
alcohol_transformed	0.294	0.018	16.695	.000	0.260	0.329	0.549
sulphates_transformed	1.255	0.130	9.680	.000	1.000	1.509	0.184
volatile acidity_transformed	-1.029	0.121	-8.474	.000	-1.267	-0.791	0.141
pH_transformed	-0.634	0.136	-4.679	.000	-0.900	-0.368	0.043
total sulfur dioxide_transformed	-0.003	0.001	-4.461	.000	-0.005	-0.002	0.039
chlorides	-3.383	0.890	-3.803	.000	-5.128	-1.638	0.028
free sulfur dioxide_transformed	0.005	0.002	1.990	.047	0.000	0.009	0.008
citric acid_transformed	-0.228	0.123	-1.852	.064	-0.469	0.013	0.007

Estimating best model without overfitting

- How to choose between different models/algorithms?
- Idea is to use “prediction quality” (e.g. SS) to assess what level of complexity is best given a particular dataset
- But we can’t use the same data we fit the model to in order to assess how well it did – could be perfect fit but not generalize to other data – each model is subject to overfitting – e.g., in genetics project we have > 6500 candidate genes but only 72 observations!
- So we deliberately leave data aside for “testing”…

Training/Test

- Randomly split data into training and test sets (often ~2/3 for train, 1/3 for test)
- Build a regression model using the *training* set and evaluate it using the *test* set
- Best if you have a lot of instances/observations (at least 100, preferably > 1000)
- Alternative when data set is not so big is to use *cross-validation* – discuss in later lecture
- Need a metric by which to evaluate…

Evaluation of best model

- Possible evaluation measures in Modeler:
  - Correlation -- correlation coefficient between the observed target values and model estimated target values
  - Relative Error $(1- R^2)$
  - Number of fields – number of variables included in the model – “smaller will be simpler model with less chance of overfitting”

Thursday's Lecture

- IBM Demo – Auto Numeric Node
- The classification prediction problem
  - Logistic regression
  - Classification trees
  - Support Vector Machines