Variable selection

Does it matter from a machine learning perspective?

Filippo Biscarini
Senior Scientist
CNR, Milan (Italy)

Traditional statistics

Two groups of pigs: diet A, diet B → which promotes growth better?

weight = mean + diet + e

Diet A	Diet B
90 kg	89 kg
88 kg	82 kg
92 kg	79 kg
87.5 kg	83 kg
…	…

!! is “diet” relevant/significant for growth?

Traditional statistics

What about the sex of the pigs? And their age? Or breed? Interactions?

weight = mean + diet + sex + e

weight = mean + diet + sex + age + e

weight = mean + diet + sex + age + breed + e

weight = mean + diet + sex + age + breed + … + e

weight = mean + diet + sex + age + breed + age*breed + … + e

Diet A	Diet B
90 kg	89 kg
88 kg	82 kg
92 kg	79 kg
87.5 kg	83 kg
…	…

What about machine learning?

In machine learning **the model learns on its own** which variables to use and how (not easily accessible by humans) → "black box"

What about machine learning?

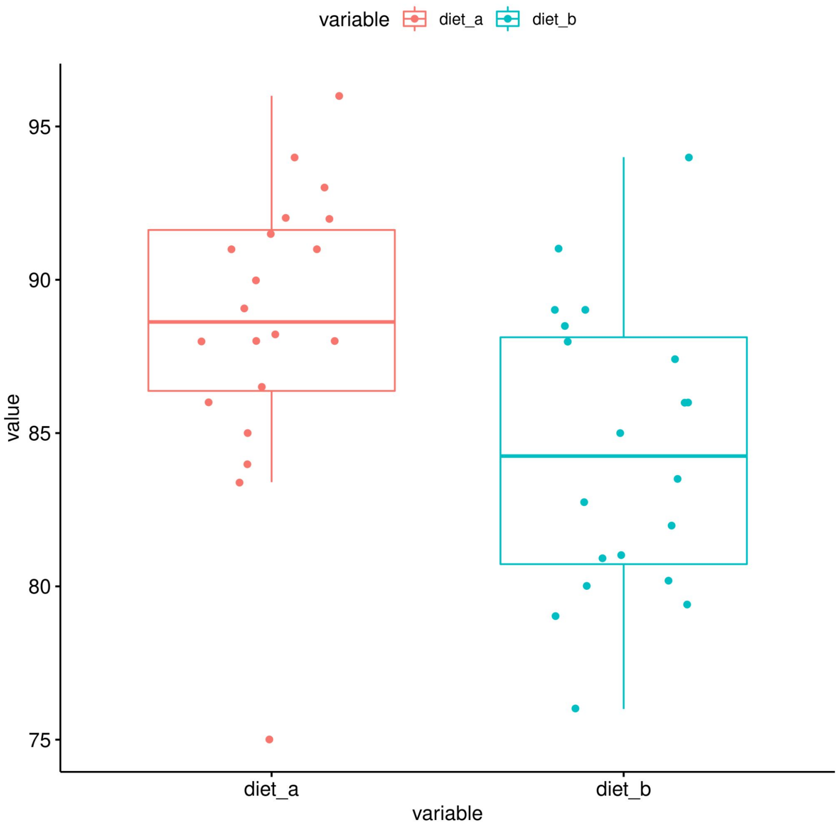
In machine learning **the model learns on its own** which variables to use and how (not easily accessible by humans) → ”black box”

- If the ML model is able to determine that burying ground quartz stuffed into the horn of a cow (which are said to harvest "cosmic forces in the soil") has no effect on the growth of pigs, this information is kept hidden in the model
- Sounds suboptimal, but **the interpretability of single variables loses sense as the number of variables** and their combinations and transformations **increases**
- And in modern statistics we usually have A LOT of variables!

An illustration - ANOVA

*term	SS	d.f.	F	p-value
intercept	189.2	1	415.11	5.2e-37
diet	2.35	1	5.39	0.022
residual	4.79	100		

*made up numbers!!

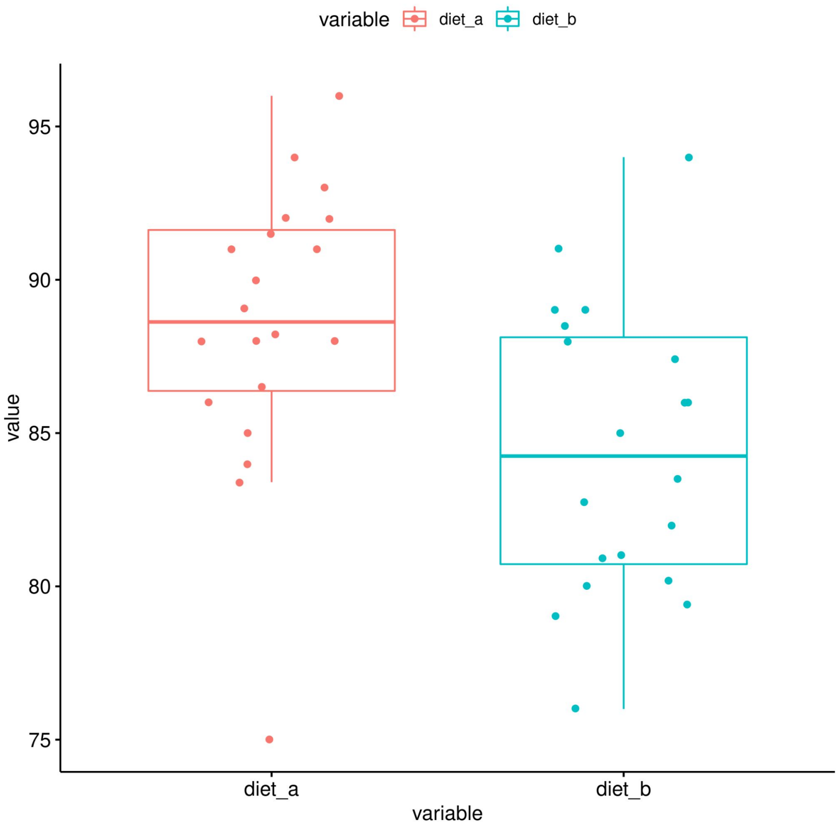


An illustration - linear model

*term	SS	d.f.	F	p-value
intercept	189.2	1	415.11	5.2e-37
diet	2.35	1	5.39	0.022
residual	4.79	100		

=

weight = mean + b1*diet + e



An illustration - linear model

weight = mean + b1*diet + e

*mean = **80** kg
*b1 = **+2.75** kg [coding diet A = 1; diet B = 0]

Interpretation

- mean: average weight of pigs
- b1: average difference in weight between pigs fed with diet A and pigs fed with diet B

***made up numbers!!**

An illustration - linear model

weight = mean + b1*diet + b2*age + e

mean = **80** kg
b1 = **+2.75** kg [coding diet A = 1; diet B = 0]
p-value = 0.006 → b2 = **+1.47** kg [coding age in years]

Interpretation

- mean: average weight of pigs
- b1: average difference in weight between pigs fed with diet A and pigs fed with diet B (at constant age)
- b2: average weight gain per year of age, keeping diet constant

made up numbers!!

An illustration - linear model

Traditional statistics approach!

weight = mean + b1*diet + b2*age + b3*motion_time + e

The coefficient for “motion time” (b3) has a p-value of 0.29: we decide not to include motion time in the model

But what if the relationship between motion time and weight is not linear?
We can fit **polynomial terms**! (square, cube etc.) [→ this is still a linear model!]

An illustration - linear model

$$\text{weight} = \text{mean} + b1{*}\text{diet} + b2{*}\text{age} + b3{*}\text{motion\_time} + b4{*}\text{motion\_time}^2 + b5{*}\text{motion\_time}^3 + e$$

The p-values for the polynomial terms are now 0.075, 0.051 and 0.032:

- **should we include these in the model?**

The coefficients for the polynomial terms are: -1.57, 0.24 and -0.03

- **how should we interpret these?**
- on average, we lose 1.57 kg per hour of motion, we gain 0.24 kg per hour-of-motion squared, and we lose 30 grams per hour-of-motion cubed

How to build and interpret the model becomes more and more confused

The machine learning perspective

With many variables (but already with a handful of variables) it becomes a titanic task to decide which variables, combinations of variables and functions of variables to include in the model
→ **let the model decide!**

The questions of variable selection and model interpretability become ill-posed
→ **predictions matter more than inference!**

Is this the end of the story? Can we really say nothing about why our model works (or does not work)?
→ **don't panic, we'll be able to crack the black box (at least partially)**

["The Return of Variable Selection": **explainable AI/ML**]

The machine learning perspective

variable selection ≠ data representation

variable selection ≠ feature extraction/engineering

How does the model decide which variables to use? (hold on a little longer …)