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Statistical modelling

Example empiricalstatistical model? Us this a correct model? Why build statistical models? Empiricalstatistical vs. data mining models Selecting a model

Abuses

Not clearly specifying the appulation Making inferences from non-probability samples Confusing the sample and population Confusing internal and external model evaluations Correlation vs. causation

Uses and abuses of statistics in geography

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Contents

Uses and abuses of statistics in geography

> David G Rossiter

Statistical modelling

Example empiricalstatistical model Is this a correct model? Why build statistical model Empiricalstatistical vs. dat mining models

Selecting a mode form

Abuses

Not clearly specifying the population Making inferences from non-probability samples Confusing the sample and population Confusing internal and external model evaluations Correlation vs. causation

Conclusions

Statistical modelling

Example empirical-statistical model Is this a correct model? Why build statistical models? Empirical-statistical vs. data mining models Selecting a model form

Abuses

Not clearly specifying the population Making inferences from non-probability samples Confusing the sample and population Confusing internal and external model evaluations Correlation vs. causation

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Statistical modelling

- Example empiricalstatistical model Is this a correct model? Why build statistical models? Empiricalstatistical vs. data mining models Selecting a model
- Abuses
- Not clearly specifying the population Making inferences from non-probability samples Confusing the sample and population Confusing internal and external model evaluations Correlation vs. causation
- Conclusions

What do we mean by "statistics"?

- Descriptive statistics 描述性统计: numerical summaries of datasets 数据集
 - Minimum, maximum, range, median, quantiles, histograms, scatterplots . . .
 - "20% of the **samples** 样本 had heavy metal values greater than the legal limit for polluted soils"
- · Inferential statistics 统计推断: quantitative statements about some population 全部
 - · with uncertainty 不确定
 - · '20% (±5% one standard error 标准误差) of the **study area** has soils with heavy metal values greater than the legal limit for polluted soils"

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Statistical modelling

Example empiricalstatistical model Is this a correct model? Why build statistical models? Empiricalstatistical vs. data mining models Selecting a model form

Abuses

Not clearly specifying the population Making inferences from non-probability samples Confusing the sample and population Confusing internal and external model evaluations Correlation vs. causation

Conclusions

Components of an empirical-statistical model

"Empirical-statistical" 经验统计: parameterized equation: dependent ~ independent variables

1 Predictand, "dependent" variable 因变量

· known at **calibration** 校准 observations (locations, times ...)

2 Predictors 独立变量, "independent" variables 自变数

- · for model building 模拟建造, also known at calibration observations
- · for prediction 预测, also known at prediction locations, times ...
- 3 Model form 模拟类型 relating predictors and predictand
- Model parameters 模拟参数 from calibration 模拟校准
- 5 Model evaluation 模拟评价: fitness for use

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Statistical modelling

Example empiricalstatistical model

Is this a correc model?

Why build statistical models' Empiricalstatistical vs. data mining models Selecting a model

Abusas

Not clearly specifying the population Making inferences from non-probability samples Confusing the sample and population Confusing interna and external model evaluations Correlation vs. causation

Conclusions

Example dataset - Meuse River (NL) heavy metals 荷兰默兹河重金属数据

predictand log(Zn) 锌对数 concentration in topsoil predictors: (1) distance to river; (2) elevation





Possible research questions

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Statistical modelling

Example empiricalstatistical model

Is this a correct model?

statistical model: Empiricalstatistical vs. dat mining models

Selecting a mode form

Abuses

Not clearly specifying the population Making inferences from non-probability samples Confusing the sample and population Confusing internal model evaluations Correlation vs. causation What proportion of the study area has heavy metal concentrations over regulatory thresholds? 管理限制
 → limits land use

2 Where are the polluted areas? → map = predict at unsampled locations

3 What are the sources 根源 of the metal?

- · Atmospheric deposition (e.g., from smelters 熔炉)?
- · River floods 洪水?
 - · Pre-industrial, from parent rock 母质 upstream
 - · Post-industrial, from industry upstream
- · (Soils are from river alluvium 冲积层, none from bedrock 基岩)

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Statistical modelling

Example empiricalstatistical model

Is this a correct model? Why build statistical model Empiricalstatistical vs. dat

statistical vs. dat mining models Selecting a mode form

Abuses

Not clearly specifying the population Making inferences from non-probability samples Confusing the sample and population Confusing internal and external model evaluations Correlation vs. causation

Relation of predictand to predictors





linear?

as square root?

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Statistical modelling

Example empiricalstatistical model

Is this a correc model?

Why build statistical models? Empiricalstatistical vs. data mining models Selecting a model form

Abuses

Not clearly specifying the population Making inferences from construction Confusing the sample and population Confusing internal and external model evaluations correlation vs. causation

Example empirical-statistical model

Multiple linear regression 多重线性回归, coefficients determined by ("fit by") Ordinary Least Squares (OLS) 普通 的最小二乘法

lm(formula = log(zinc) ~ elev + sqrt(dist), data = meuse)

Residuals:

Min 1Q Median 3Q Max -0.99144 -0.22853 0.00209 0.22244 0.98324

Coefficients:

Estimate Std. Error t value Pr(>|t|)(Intercept)8.641570.2520634.284< 2e-16</td>***elev-0.232170.03426-6.7772.54e-10***sqrt(dist)-1.977660.16025-12.341< 2e-16</td>***

Multiple R-squared: 0.7226, Adjusted R-squared: 0.7189

Interpretation

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Statistical modelling

Example empiricalstatistical model

Is this a correc model?

Why build statistical models Empiricalstatistical vs. data mining models Selecting a model

Ahuses

Not clearly specifying the population Making inferences from non-probability samples Confusing the sample and population Confusing internal model evaluations Correlation vs.

1 An additive linear model

- log(Zn) changes linearly with elevation and linearly as the square root with distance to river
 - supports the theory that the heavy metal orginates in flood water (higher, further from river \rightarrow less pollution)
- · no interaction 相互独立 between predictors
- 2 Residuals 残差 are lack of fit; almost ±1 log(Zn)
- 3 Coefficients 系数 show the effect of each predictor; each has a standard error (uncertainty)
- ④ Model explains 71.9% of the total varibility 总变量 in the sample set

Is this a correct model?

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Statistical modelling

Example empiricalstatistical model

Is this a correct model?

Why build statistical models? Empiricalstatistical vs. data mining models Selecting a model form

Abuses

Not clearly specifying the population Making inferences from non-probability sample Confusing the sample and population Confusing internal model evaluations Correlation vs. causation 1 Are the relations between predictors and predictand linear?

- 2 Are the relations independent of each other, or are there interactions 相互独立 between predictors?
- 3 Are the assumptions of linear modelling satisfied?
 - Residuals must be independent and identically-distributed residuals; as a group normally-distributed
 - Homoscedasctic 同方差 (same variance across range of predictand)
 - · No relation between fitted values 计算值 at observed points and residuals
 - · No spatial or temporal correlation 相关 among residuals
- (

4 How sucessful is the model for prediction?

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Statistical modelling

Example empiricalstatistical model

Is this a correct model?

Why build statistical models? Empiricalstatistical vs. data mining models Selecting a model form

Abuses

Not clearly specifying the population Making inferences from non-probability samples Confusing the sample and population Confusing internal model evaluations Correlation vs. Causation

Conclusions

Compare on a 1:1 (Actual:Fitted) line.



log(Zn) ~ sqrt(distance_to_river) + elevation_m.a.s.l

No relation between fitted values and residuals - good!

Residuals

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Statistical modelling

Example empiricalstatistical model

Is this a correct model?

Why build statistical models? Empiricalstatistical vs. data mining models Selecting a model form

Abuses

Not clearly specifying the appulation Making inferences from non-probability samples Confusing the sample and population Confusing internal model evaluations Correlation vs. causation

onclusions

Spatial correlation of linear model residuals

Variogram of residuals from additive linear model



Residuals are *not* independent! Closer separation in *geographic* space \rightarrow closer separation in *feature* space **This modelling assumption is not satisfied**!

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Statistical modelling

Example empiricalstatistical model

Is this a correct model?

Why build statistical models? Empiricalstatistical vs. data mining models Selecting a model form

Abuses

Not clearly specifying the population Making inferences from non-probability samples Confusing the sample and population Confusing internal and external model evaluations Correlation vs.

Conclusions

Example: Moisture content of surface soils vs. drought indexfrom remote sensing



 $R^2 = 0.585$ $R^2 = 0.445$

Linear model is incorrect! although it explains more of the variation. The relation is obviously not linear.

Q: Is the power curve 幂函线 shown in the right figure a correct model? (Does it correctly represent the **process** 过程?)

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Statistical modelling

- Example empiricalstatistical model
- Is this a correct model?
- Why build statistical models
- Empiricalstatistical vs. data mining models Selecting a model form

Abuses

Not clearly specifying the population Making inferences from non-probability samples Confusing the sample and population Confusing internal and external model evaluations Correlation vs. Causation

Conclusions

Why do we build statistical models?

● To (partially) **understand** 理解 (gain insight into 深刻 了解) a **geographical process** 地理的过程

- The **form** of the model suggests the form of the process
- The **parameters** of the model suggest the influence of predictors
- The **evaluation** of the model suggest how well the model fits the process
- 2 To predict unobserved locations (mapping 地图绘制) or times (forecasting) or cases (future observations)
 - Apply the model to cases or locations or times, if we know the values of the **predictor** variables
 - Predict with **uncertainty** derived from the model evaluation

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Statistical modelling

Example empiricalstatistical model

Is this a correct model?

Why build statistical models

Empiricalstatistical vs. data mining models

Selecting a model form

Abuses

Not clearly specifying the population Making inferences from non-probability samples Confusing the sample and population Confusing internal model evaluations Correlation vs. causation Empirical-statistical vs. data mining models

Empirical-statistical 实验性的统计模拟 give an explicit model 明确的 which can be examined for insight into processes and for prediction

> • Examples: multiple (linear) regression, principal components (PCA), discriminant analysis, logistic regression . . .

Data mining 数据挖掘 purely **data driven**, useful for prediction but give little insight into process; "black" (or maybe "grey") box models

> • Examples: Random forests (RF) 随机森林, artificial neural networks (ANN), support vector machines (SVM)...

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Statistical modelling

Example empiricalstatistical model

Is this a correct model?

Why build statistical model

Empiricalstatistical vs. data mining models

Selecting a model form

Abuses

Not clearly specifying the population Making inferences from non-probability samples Confusing the sample and population Confusing internal and external model evaluations Correlation vs.

Example data mining model - Regression tree 回归树

Meuse River soil heavy metals dataset

Interpretation

Uses and abuses of statistics in geography

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Statistical modelling

Example empiricalstatistical model

ls this a correct model?

Why build statistical models

Empiricalstatistical vs. data mining models

Selecting a model form

Abuses

Not clearly specifying the population Making inferences from non-probability samples Confusing the sample and population Confusing internal and external model evaluations Correlation vs. causation

- 155 observations, mean concentration 平均浓度 log(Zn) = 2.56 mg kg⁻¹
- Split dataset into two parts, based on distance to river = 145 m; each group with its own mean value
 - \cdot < 145: 54 observations, mean 2.87 mg kg⁻¹
 - \cdot >= 145: 101 observations, mean 2.39 mg kg⁻¹
 - This is the maximum reduction in within-group variance 组内方差, maximum increase in between-group variance 相组方差
- Gontinue to split until improvement in variance is "small"
- This is purely empirical, putting observations into "boxes", no statistical model is used

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Statistical modelling

Example empiricalstatistical model

Is this a correc model?

Why build statistical mode

Empiricalstatistical vs. data mining models

Selecting a model form

Abuses

Not clearly specifying the population Making inferences from non-probability samples Confusing the sample and population Confusing internal and external model evaluations Correlation vs. causation

Conclusions

Example data mining model - Random forest 随机森林

Use a set of **many trees** with **resampling** 重新取样; predict based on all of these and average them

Calibration fit

Cross-validation fit

Variable importance 变量重要性 (increase in mean squared error under randomization): flood frequency 9%; distance to river 68%; elevation 54%

Selecting a model form

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Statistical modelling

- Example empiricalstatistical model
- Is this a correct model?
- Why build statistical models Empirical-
- statistical vs. data mining models

Selecting a model form

Abuses

Not clearly specifying the population Making inferences from non-probability samples Confusing the sample and population Confusing internal and external model evaluations Correlation vs.

- Should match what is hypothesized or known about the process based on prior knowledge
- Simpler ("parsimonious" 吝啬的) is better, don't complicate a model unless there is a substantial improvement
 - · Easier to interpret
 - More likely to give higher prediction precision 预测 准确
- Compare models based on evalution statistics, but don't change models just on this basis
- Test model form robustness 稳健性 by comparing coefficients based on fitting the model with different random sub-samples
- Mapping models: compare spatial distribution 空间 分布 of predictions with landscape features 地貌特征

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Statistical modelling

Example empiricalstatistical model Is this a correct model? Why build statistical models? Empiricalstatistical vs. data mining models

Selecting a mode form

Abuses

Not clearly specifying the population Making inferences from non-probability samples Confusing the sample and population Confusing internal model evaluations Correlation vs. causation

Conclusions

Example of competing 比较 model forms

Problem: predict topsoil soil organic matter (SOM) concentration from environmental variables

Source: Zeng, Can-Ying *et al.* (2016). *Mapping soil organic matter* concentration at different scales using a mixed geographically weighted regression method. **Geoderma**:281, 69–82.

Predictor variables

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Statistical modelling

Example empiricalstatistical model Is this a correct model? Why build statistical models? Empiricalstatistical vs. data mining models

Selecting a model form

Abuses

Not clearly specifying the population Making inferences from non-probability samples Confusing the sample and population Confusing internal and external model evaluations Correlation vs. causation

Variables Module Terrain Elevation Elevation Slope Slope in ArcInfo Planc Plan curvature (Shary et al., 2002) Profile curvature (Sharv et al., 2002) Profic TWI Topographic wetness index (Qin et al., 2009a,b) Hand Height above the nearest drainage (Gharari et al., 2011) Dand Distance to the nearest drainage (Gharari et al., 2011) TCI Terrain characterization index (Park and Van De Giesen, 2004) TPI Topographic position index (Jenness, 2005) Flowlen Flow length based on MFD (Oin et al., 2007) VallevI Valley index RPI Relative position index (Skidmore, 1990) Five binary variables based on fuzzy slope position (Qin et al., 2007) including ridge, shoulder slope (shoulder), back slope (back), foot slope (foot), channel Climate Precipitation Annual average precipitation Annual average temperature Temperature Vegetation EVIs Summer average EVI **EVIa** Annual average EVI Parent materials Eight binary variables: shale, sandstone, pyroclastic rocks (pyroclastic), granite and granodiorite, limestone, conglomerate, quaternary clay-silt-gravel (clay-silt-gravel), quaternary vermicule boulder and grave clay (grave clay)

These are all known to affect SOM concentration, via various **processes** \rightarrow **model** reflects **reality** *Example*: higher elevation \rightarrow cooler temperatures, more rainfall, less evapotranspiration \rightarrow slower decomposition of SOM

Candidate model forms

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Statistical modelling

- Example empiricalstatistical model
- Is this a correct model?
- Why build statistical models Empiricalstatistical vs. data
- Selecting a model form

Abuses

- Not clearly specifying the population Making inferences from non-probability samples Confusing the sample and population Confusing internal and external model evaluations Correlation vs.
- Conclusions

- Multiple linear regression (MLR); select the "best" set of predictors
- Principal components regression (PCR); predictor set is reduced by Principal Compents Analysis (PCA)
- Ordinary Kriging (OK): predict only from known points, ignore predictor variables
- 4 Kriging with an External Drift (KED): MLR with OK of the residuals from MLR
- **5** Geographically-weighted regression (GWR): like MLR, but coefficients can **vary** across the area
- 6 GWR-K: GWR with OK of the residuals
- 7 many more! 等等

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Statistical modelling

- Example empiricalstatistical model
- Is this a correct model?
- Why build statistical models Empiricalstatistical vs. dat
- Selecting a model form

Abuses

Not clearly specifying the population Making inferences from non-probability samples Confusing the sample and population Confusing internal model evaluations Correlation vs. causation

Conclusions

Processes implied by these models

1 MLR: covariates **linearly** affect predictand

- variation: transform predictors or predictands, e.g., log-linear relation
- 2 PCR: same, but removes colinearity among predictors
 → identifies latent factors
- 3 OK: predictors are not useful, SOM does not depend on the covariates, only local spatial correlation 空间 自相关
- 4 KED: some variation is explained *globally* as in MLR but residual variation has *local* spatial dependence
- **5** GWR: covariates linearly affect predictand, but the strength of the relation changes over the area
- **6** GWR-K: some variation is explained as in GWR-K but residual variation has local spatial dependence

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Statistical modelling

Example empiricalstatistical model Is this a correct model? Why build statistical models Empiricalstatistical vs. data

Selecting a model form

Abuses

Not clearly specifying the population Making inferences from non-probability samples Confusing the sample and population Confusing internal and external model evaluations Correlation vs. causation

Conclusions

Question: which model best corresponds to the physical process?

· Soil geographers have a well-developed theory:

$$s_0 = f(s, c, o, r, p, a, n)$$

 s_0 : soil property to be predicted right-hand side: other soil observations climate, organisms, relief, parent material, age, neighbourhood

- But the **functional form** of this equation is not determined by theory
- Many studies of each factor separately (e.g., *chronosequence, toposequence...*), a few of interactions, none of the complete equation
- We would like our model to correspond to the physical processes by which these factors produce soil.

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Statistical modelling

Example empiricalstatistical model Is this a corre

Model? Why build statistical models Empiricalstatistical vs. data mining models

Selecting a model form

Abuses

Not clearly specifying the population Making inferences from non-probability samples Confusing the sample and population Confusing internal model evaluations Correlation vs. causation

Conclusions

Comparing mapping results - side-by-side

Fig. 7. The distribution of A-horizon soil organic matter maps based on the different model of group 2 for Heshan farm.

Look for **details of soil-landscape** relation. E.g., small valleys \rightarrow high moisture \rightarrow higher SOM.

"Correct" (or at least plausible) spatial pattern \rightarrow confidence that the model is correct

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Statistical modelling

Example empiricalstatistical model

Is this a correct model?

Why build statistical models? Empiricalstatistical vs. data mining models

Selecting a model form

Abuses

Not clearly specifying the population Making inferences from non-probability sample Confusing the sample and population Confusing internal model evaluations Correlation vs. causation

Comparing mapping results - difference maps

Choice of model form has a large influence on the map!

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Statistical modelling

Example empiricalstatistical model

Is this a correct model?

Why build statistical models Empirical-

statistical vs. data mining models

Selecting a model form

Abuses

Not clearly specifying the population Making inferences from non-probability samples Confusing the sample and population Confusing internal and external model evaluations Correlation vs. causation

Conclusions

Evidence that a model form is suitable

1) internal 模拟内: from the model itself:

- how well the model fits the data (success of calibration);
- how well the fitted model meets the model assumptions
- 2 external 模拟外 to the model:
 - what is known or suspected about the process in the real world that gave rise to the data (what we measure and observe)
 - e.g., atmospheric pressure decreases (linearly ?) with altitude; fewer molecules hold less heat
 - so, we observe cooler temperatures as we move up a mountain
 - how well the model fits observations from the target population
 - · success of evaluation ("validation" 证实) with:
 - an independent dataset
 - a simulated independent set by resampling ("cross-validation" 交互证实, "bootstrapping", "jackknifing")

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Statistical modelling

- Example empiricalstatistical model
- Is this a correct model?
- Why build statistical models Empiricalstatistical vs. data mining models
- Selecting a model form

Abuses

Not clearly specifying the population Making inferences from non-probability sample Confusing the sample and population Confusing internal model evaluations Correlation vs. causation

Common abuses and misunderstandings of statistics

Not clearly specifying the population

2 Making inferences from unrepresentative samples

- · Confusing populations with samples
- Confusing **descriptive** and **inferential** statistics from a set of observations

3 Internal vs. external model evaluation

- 1:1 predicted vs. actual, different from linear regression for model evaluation
- 4 Correlation vs. causation; lurking variables

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Statistical modelling

Example empiricalstatistical model

Is this a correc model?

Why build statistical model Empirical-

statistical vs. dat mining models

Selecting a model form

Abuses

Not clearly specifying the population

Making inferences from non-probability samples Confusing the sample and population Confusing internal and external model evaluations Correlation vs. causation

Conclusions

Abuse: Not clearly specifying the population

- We make inferences 推断的结果 about a population 全部 from a sample 样本 taken from it
 - $\cdot\,$ e.g., map the soil properties in an area, from observations within it
- The sample must cover "all" the variation in the **target** population the one we want to make statements about.
- Dangerous to extrapolate 外推 beyond the limits of the population of which the sample is representative 典型的
 - geographic area; but can argue that the **geographic context** in the extrapolation area matches the calibration area (same climate, same geology ...)
 - range of measured attributes; no way to know if the relation holds beyond this range

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Statistical modelling

Example empiricalstatistical model Is this a correct model? Why build statistical models? Empiricalstatistical vs. data mining models

form

Abuses

Not clearly specifying the population

Making inferences from non-probability samples Confusing the sample and population Confusing internal and external model evaluations Correlation vs. causation

Conclusions

Interpolation 内推 vs. Extrapolation 外推

Figure 1 The winning Olympic 100-metre sprint times for men (blue points) and women (red points), with superimposed best-fit linear regression lines (solid black lines) and coefficients of determination. The regression lines are extrapolated (broken blue and red lines for men and women, respectively) and 95% confidence intervals (dotted black lines) based on the available points are superimposed. The projections intersect just before the 2156 Olympics, when the winning women's 100-metre sprint time of 8.079 s will be faster than the men's at 8.098 s.

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Statistical modelling

Example empiricalstatistical model Is this a correct model? Why build statistical models? Empiricalstatistical vs. data mining models Selecting a model form

Abuses

Not clearly specifying the population

Making inferences from non-probability samples Confusing the sample and population Confusing internal and external model evaluations Correlation vs. causation

Conclusions

Example study area - what is the population?

Purpose:

(1) **map** polluted soils in flood plain of Meuse (Maas) River, NL 荷兰

(2) infer source of pollution (upstream industry? aeolian? parent rock?)

Belgium 比利时 on the left bank of river; also flooded.

Is this in the target population? Does the sample allow us to say anything about it?

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Statistical modelling

Example empiricalstatistical model

model? Why build statistical models? Empiricalstatistical vs. data mining models Selecting a model form

Abuses

Not clearly specifying the population

Making inference from non-probability samples

Confusing the sample and population

Confusing internal and external model evaluations Correlation vs. causation

Conclusions

Abuse: Making inferences 推断的结果 from non-probability 不概率 samples

Population a set of elements (individuals) about which we want to make a statement Sample a subset of elements taken from a

population

What is the relation of the sample to the population?

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Statistical modelling

Example empiricalstatistical model Is this a correct model? Why build statistical models Empiricalstatistical vs. dat

Selecting a model form

Abuses

Not clearly specifying the population

Making inference from non-probability samples

Confusing the sample and population Confusing inter

and external model evaluations Correlation vs. causation

Conclusions

Relation of the sample to the population

Opportunistic sample 机会样本 See it, grab it; no system; easy access; e.g., sample soils in roadcuts

Purposive sample 故意样本 Select elements based on expert knowledge; e.g.,"typical" ("modal") landscape position to sample soils

"Representative" sample 典型样本 the "expert's" assessment of the purposive sample, no way to check

Probability sample 概率样本 Enumerate all elements that could be sampled ("sampling frame") and use a **random** selection

> completely random, stratified 分层 random, cluster 成群的 sampling, two-stage ...

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Statistical modelling

Example empiricalstatistical model Is this a correct model? Why build statistical models? Empiricalstatistical vs. data mining models Selecting a model form

Abuses

Not clearly specifying the population Making inferences from non-probability samples

Confusing the sample and population

Confusing internal and external model evaluations Correlation vs. causation

Conclusions

Sample "20% of the samples had heavy metal values greater than the legal limit for polluted soils"

Population "20% (±5% one standard error 标准误差) of the soils **in the study area** have heavy metal values greater than the legal limit for polluted soils"

The first (sample) is always valid: **descriptive** statistics.

The second (population) is only valid for a **probability sample**. It also allows the computation of **confidence limits** 置信区间 or **credible intervals** 可信区间 for the population.

Population vs. sample statistics

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Statistical modelling

- Example empiricalstatistical model Is this a correc model?
- Why build statistical model: Empiricalstatistical vs. dat mining models
- Selecting a model form

Abuses

Not clearly specifying the population Making inferences from non-probability samples

Confusing the sample and population

Confusing internal and external model evaluations Correlation vs. causation

- Sample: what was observed descriptive statistics always valid:
 - > summary(meuse\$zinc)

Min. 1s	t Qu.	Median	Mean 3rc	l Qu.	Max.
113	198	326	470	674	1840

- **Population**: what are the true values of the population? Must **infer**.
- Was the sample a **probability sample?** Use a t-distribution of the mean
 - > t.test(meuse\$zinc)
 95 percent confidence interval: 411.47 527.96
 sample estimates: mean of x: 469.72
- Not a probability sample → use a geostatistical model (other assumptions!)

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Statistical modelling

Example empiricalstatistical model Is this a correct model? Why build statistical models? Empiricalstatistical vs. data mining models Selecting a model form

Abuses

Not clearly specifying the population Making inferences from non-probability samples Confusing the sample and population Confusing internal and external

Correlation vs. causation

Conclusions

Abuse: Confusing internal and external model evaluations

Internal 内边 Only using the same **calibration** data that was used to build the model

• Often **too optimistic**; try to minimize by using measures that account for

External 外边 Using independent evaluation ("validation") data

- Must be a **probability** sample from the target population
- Can be "pseudo-independent": a simulated independent set by resampling (cross-validation, bootstrapping) if the original sample was a probability sample

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Statistical modelling

Example empiricalstatistical model Is this a correct model? Why build statistical models Empiricalstatistical vs. data mining models Selecting a model form

Abuses

Not clearly specifying the population Making inferences from non-probability samples Confusing the sample and population Confusing internal and external model evaluations

Correlation vs. causation

Conclusions

Model calibration vs. evaluation

Calibration 模拟校准 finding "best" values of model parameters

Evaluation 模拟评价 assessing the usefulness of the model for its purpose; fitness for use

• "Validation" 证实 statistics (RMSE etc.) must be placed in context

Example of internal model fit

Not clearly specifying the population Making inferences from non-probability samples Confusing the sample and population Confusing internal and external model evaluations

Correlation vs. causation

Conclusions

Distance to 1:1 line is the **residual** from the fit; i.e., unexplained by model.

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Statistical modelling

Example empiricalstatistical model Is this a correct model? Why build statistical models? Empiricalstatistical vs. data mining models Selecting a model

Abuses

Not clearly specifying the population Making inferences from non-probability samples Confusing the sample and population Confusing internal and external model evaluations

Correlation vs. causation

Conclusions

Example external evaluation: leave-one-out cross-validation

Each observation is predicted by a model built from the other observations.

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Statistical modelling

Example empiricalstatistical model

Is this a correct model?

Why build statistical models? Empiricalstatistical vs. data mining models Selecting a model

Abuses

Not clearly specifying the population Making inferences from non-probability samples Confusing the sample and population Confusing internal

and external model evaluations

Correlation vs. causation

Conclusions

Abuse: 1:1 vs. linear regression for model evaluation

Compare a model **predictions** with **observations**:

● Compare 1:1 一比一的线 Actual:Predicted 真实的:预测的- this tells how good the model is

- · If cross-validation or independent evaluation sample, a good measure of **predictive precision**
- 2 Linear regression of Actual on Predicted this tells how much gain 增益 and bias 偏移 is in the model.

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Statistical modelling

Example empiricalstatistical model Is this a correct model? Why build statistical models? Empiricalstatistical vs. data mining models

SOC % (Wakely-Black)

Selecting a mo form

Abuses

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Rwanda SOC lab. duplicate analyses

SOC % (loss on ignition)

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Statistical modelling

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Abuses

Not clearly specifying the population Making inferences from non-probability samples Confusing the sample and population Confusing internal model evaluations **Correlation vs. Correlation vs.** Abuse: Correlation/regression 相互关系/回归 vs. causation 原因; lurking variables 潜藏变量

- We may have a good **statistical** relation between one or more predictors *X* and a predictand (target) *y*.
- But this does not mean that, in the real world, X causes or influences y.
 - That is a **meta-statistical** argument, from **physical principles** and experiment.
- Example: good correlation between two lab. tests of the same property does one "cause" the other?
 - · No! The "**lurking variable**" 潜藏变量 here is the physical nature of the property itself
 - The statistical relation can be used to translate from one test to the other, with no concept of causation

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Statistical modelling

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Not clearly specifying the population Making inferences from non-probability samples Confusing the sample and population Confusing internal and external model evaluations **Correlation vs. causation** Example: Correlation vs. causation

- Plant growth modelled as a function of temperature, rainfall and soil nutrient levels - do these cause or at least influence the plant growth?
 - Yes, we know this from lab. experiments.
- Growing season length modelled as a function of crop yield - is there a causative relation?
 - No, the cause is the other direction. But this model could be useful for interpolating growing season in areas with no direct temperature measurements, but where crop yield is measured.

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- Statistical models allow us to make inferences about populations, from samples taken from the population
 - These inferences include (1) insight into the processes in nature; (2) predictions
- Models must have an appropriate form, be properly calibrated, and evaluated for their fitness for use

End

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Conclusions

尽管还难以达到百分之百的准确,我们仍要尽百分之百的努力。 We are not perfect, but we will do our best

(来原:上海气象局)

尽管还难以达到百分之百准确,我们仍要尽百分之百努力。 "Although it is still difficult to achieve complete accuracy, we will still give full effort."