

Quantifying prediction accuracy

Context: Using leave-one-out (loo) cross-validation

PRESS statistic: Prediction Residual Error Sums-of-Squares

loo idea, quantifying overall accuracy predicting new observations

like Sum-of-squared errors but quantifies prediction accuracy

$$\text{PRESS} = \sum_{\text{obs}} (Y_i - \hat{Y}_{-i})^2$$

\hat{Y}_{-i} is prediction of Y_i from model fit without Y_i

Almost always larger than $\text{SSE} = \sum_{\text{obs}} (Y_i - \hat{Y}_i)^2$

Because PRESS prediction of Y_i not based on Y_i

Things we haven't covered that are of general interest

Paired yes/no data

Regression with count responses

Flexible regressions (Splines, CART, Random Forests)

Two-way factorial ANOVA

Randomized Complete Block Designs (RCBD) Quick introduction to these topics

Goal is that you know some names if you want to pursue any topic

Stat 5710 (Intro to Expt. Design) covers factorial ANOVA and RCBD in great depth

Paired yes/no data:

Vit C study: what if conducted differently?

Find households with 2 adults.

Within each household, one adult gets Vit C, other gets Placebo

Data are paired (yes/no response doesn't change that aspect of the design)

My experience is that this pairing often gets forgotten

Chi-square test is wrong (obs. are not independent)

se of log odds ratio is wrong

There are methods that explicitly account for pairing

analog of the paired t-test for continuous responses

one simple one is McNemar's test

Regression with count responses

Two types:

Fixed maximum: Binomial distribution

unlimited maximum: Poisson distribution

Example: Case study 22.1: African elephant matings

Q: Do older elephants have more successful matings

Does success of elderly elephants "slow down"?

Poisson distribution:

Statistical model for non-negative counts

One parameter: mean. Variance is the same as the mean

So, samples from a Poisson distribution with larger mean have larger standard deviation

$\lambda = \text{mean} \geq 0$, doesn't have to be an integer (2.2 children in the average family)

Relate λ to covariates by:

$$\log \lambda_i = \beta_0 + \beta_1 X_{1i} + \beta_2 X_{2i} \cdots$$

Increasing X_{1i} by 1 multiplies λ by $\exp \beta_1$

Elephant example: plots linked to graphs page

Data exploration:

Mean # matings increases with age,

Pattern seems linear when $Y = \log(\# \text{ matings})$

SD # matings also increases with age

Q: Do older elephants have more successful matings?

Fit a Poisson regression model with linear predictor, log link:

$$\begin{aligned} \log \lambda_i &= \beta_0 + \beta_1 \text{Age}_i \\ Y_i &\sim \text{Poisson}(\lambda_i) \end{aligned}$$

Estimated coefficients (se):

Intercept: -1.582 (0.545)

Slope: 0.0687 (0.0138)

Interpretation of slope:

Mean # matings for an elephant that is 1 year older is 7.1% larger than that for the younger elephant

$$\exp 0.0687 = 1.071$$

Interpretation of slope - 2nd version with 10 year change:

Mean # matings for elephant approximately doubles when comparing an individual to one that is 10 years younger.

$$\exp(10 \times 0.0687) = 1.988$$

Q: Does success of elderly elephants “slow down”?

Write a model that allows that, e.g., quadratic

$$\begin{aligned} \log \lambda_i &= \beta_0 + \beta_1 \text{Age}_i + \beta_2 (\text{Age}_i)^2 \\ Y_i &\sim \text{Poisson}(\lambda_i) \end{aligned}$$

$$\hat{\beta}_2 = -0.00086, \text{ se} = 0.002, \text{ p} = 0.67$$

No evidence that increase in success “slows down” in elderly elephants

Comments about Poisson regression

Why is conclusion about mean instead of median?

Model is a log transformation of the mean (λ_i) not of the data values (Y_i)

Why not just log transform # matings and use SLR? Various reasons

Poisson regression accommodates 0 values

$\log 0$ undefined \rightarrow problem when $Y_i = 0$

0 values are no problem so long as $\lambda > 0$, $\lambda = 0.000001$ is just fine

Regression problems: λ never = 0

ANOVA problems: Can get $\lambda = 0$ when all observations in a group are 0

Detail: different relationship between mean and sd

Detail: $\log Y_i$ is not normally distributed, e.g., values are $\log 1$ or $\log 2$

Overdispersion in models for count data:

Both Binomial and Poisson distributions: $\text{Var } Y_i$ depends on mean Y_i i.e., π_i or λ_i

Sometimes the data are more variable than they “should” be

This is known as overdispersion

Account for it by using a more complicated distribution for the data

Fixed maximum: Beta binomial distribution instead of Binomial

Unlimited maximum: Negative binomial distribution instead of Poisson

My experience is that most ag/bio count data is overdispersed

Analysis of these data must account for overdispersion

Only exception is bird eggs/clutch, which are less variable than expected

Smoothing splines:

Goal: model relationship between Y and X without specifying the details

We’ve seen linear: $E Y_i = \beta_0 + \beta_1 X_i$ and quadratic $E Y_i = \beta_0 + \beta_1 X_i + \beta_2 X_i^2$ models

If curve needs to bend in a different way, could use higher order polynomial models

Adding more terms allows curve to “wobble” more.

But only in the ways “allowed” by some specific polynomial

Smoothing splines let the data tell the model where/how much to bend

Model is

$$Y_i = f(X_i) + \varepsilon_i$$

where $f(X_i)$ is an arbitrary function estimated from the data

Simple model is a series of line segments joined together

bends where data bends, straight where data straight

Continuous, but not smooth (1st and 2nd derivatives not continuous)

More useful: join cubic polynomials that are continuous

with continuous 1st and 2nd derivatives

Looks smooth, most common choice for splines

Practical issue: how wiggly is the fitted curve?

A model selection issue: want to fit the data, but not overfit

A curve that wiggles a lot probably overfits the data

Common solution: borrow a model selection idea

combine Fit + penalty for wiggleness (= complexity)

What can this be used for?

Learning: understand relationship between Y and X

Interpolation: predict Y for X 's inside the data

Splines do not extrapolate well (no data to estimate the curve)

Evaluate a specific model

Overlay predicted values from the model and from a spline

CART models: Classification and Regression Trees

Really useful for multiple X variables with complicated interaction effects

Predictor is a dichotomous key like classifying species

Model (for Gaussian data): $Y_i = f(X_i) + \varepsilon_i$, $\varepsilon_i \sim N(0, \sigma^2)$

Like splines: estimate $f(X)$ from data

but prediction is the average of a group of observations

Example from SAT data: if $Itakers \geq 3.205$, predict 877.4; if not, predict 1002

Those values are the means of the groups with $Itakers \geq 3.205$ and $Itakers < 3.205$

Algorithm:

Consider all variables, and all possible split points

Find the variable and split point that best separates two groups

details of “best” depend on nature of the data (continuous, count, yes/no)

Split the data, consider each subgroup separately

Find the best split for subgroup 1, result is two sub-sub-groups

And for subgroup 2, giving 2 more sub-sub-groups

Keep splitting until:

no effective split

or groups too small to split further (user specified limit)

Practical experience is that a tree tends to overfit the data

“prune” the tree by removing lowest branches

decision often made using cross-validation

Make prediction by working down the tree

at each split, decide which way the observation goes

when get to end, prediction is the average for that leaf

CART models:

require quite a bit of data (> 100 observations, >250 is better)

are really effective with contingent relationships

SAT: rank only matters when $Itakers < 3.205$

not as useful when a simple model (e.g., linear) is sufficient

Random Forest:

Extension of a CART model

Idea is to create many trees by resampling the original data

500 trees is common, often more.

Prediction: have covariate values

Use covariates to make a prediction from each model, so 500 predictions

report their average as the prediction for that observation

An example of “ensemble” prediction: using many models

Seems weird, but works extremely well

Random Forests are the best “out of the box” method to make predictions

my experience and opinion, shared by lots of others

“out of the box” means they work on lots of different types of problems

without requiring a lot of problem-specific tweaking.