Nonparametric Methods for Sample Surveys of Environmental Populations

Metodi Nonparametrici nell’Inferenza per Popolazioni Finite di carattere Ambientale

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Problem

Northeastern Lakes – EMAP surveyed ANC in 334 out of 21,026 lakes in the years 1991-1996 (some revisited). How many lakes are acidic/at risk of acidification?
How to deal with it

- It could be determined through Acid Neutralizing Capacity (ANC) thresholds
  - ANC < 200 → risk of acidification
  - ANC < 50 → high risk of acidification
  - ANC < 0 → acidified lake

⇒ ESTIMATION OF THE CDF
How to deal with it

- It could be determined through Acid Neutralizing Capacity (ANC) thresholds
  - $\text{ANC} < 200 \rightarrow$ risk of acidification
  - $\text{ANC} < 50 \rightarrow$ high risk of acidification $\Rightarrow$ ESTIMATION OF THE CDF
  - $\text{ANC} < 0 \rightarrow$ acidified lake

- Lakes are selected through a complex design from a frame of lakes $\rightarrow$ finite population approach to get the estimate and the confidence bounds

- Auxiliary information available for each lake in the frame
Formalizing the problem

- $\mathcal{U} = \{u_1, \ldots, u_N\}$ is the finite population of lakes labeled by the integers $i = 1, \ldots, N$ [$N = 21,026$ in our application];

- $y_i$ is the value taken by the survey variable $y$ [ANC] in unit $i$ [average over revisits];

- $z_i = I(y_i \leq t)$ is the indicator variable whose population mean $F_N(t) = N^{-1} \sum_{i \in \mathcal{U}} z_i$ is the parameter of interest i.e. the CDF at $t$ [$t = 0, 50, 200$];
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- \( y_i \) is the value taken by the survey variable \( y \) [ANC] in unit \( i \) [average over revisits];
- \( z_i = I(y_i \leq t) \) is the indicator variable whose population mean \( F_N(t) = \frac{1}{N} \sum_{i \in U} z_i \) is the parameter of interest i.e. the CDF at \( t \) \( [t = 0, 50, 200] \);
- \( s \) is the sample of size \( n \) drawn from \( U \) according to a probabilistic sampling plan with inclusion probabilities \( \pi_i \) and \( \pi_{ij} \) for all \( i, j \in U \) \( [n = 334] \);
- we have \( y_i \) known for \( i \in s \); the Hajek estimator for \( F_N(t) \) is

\[
\hat{F}_H(t) = \frac{\sum_{i \in s} d_i z_i}{\sum_{i \in s} d_i} = \sum_{i \in s} d_i^* z_i
\]

with design weights \( d_i = 1/\pi_i \) and \( d_i^* = d_i / \sum_{i \in s} d_i \).
Auxiliary Information

- The Hajek estimator does not employ AI.
- We have $y_i$ known for all $i \in s$ AND $x_i = (x_{1i}, x_{2i}, \ldots, x_{Qi})$ known for all $i \in U$; in particular for our application:
  
  \begin{align*}
    x_{1i} &= x\text{-geographical coordinate of the centroid of each lake}, \\
    x_{2i} &= y\text{-geographical coordinate}, \\
    x_{3i} &= \text{categorical variable for eco-region (7 levels)}, \\
    x_{4i} &= \text{elevation}
  \end{align*}

- It should be possible to improve the efficiency using AI.
AI for the estimation of a population mean: an overview

- Model based/assisted approach
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- To estimate the population mean of $y$, consider an assisting model such that $E_{\xi}(y_i) = \mu(x_i)$ and some design-based estimates $\hat{\mu}_i$:
  - GREG-type estimators $\bar{y}_G = \frac{1}{N} \sum_{i \in U} \hat{\mu}_i + \frac{1}{N} \sum_{i \in s} d_i (y_i - \hat{\mu}_i)$.
  - Calibration-type estimators $\bar{y}_C = \frac{1}{N} \sum_{i \in s} w_i y_i$ with weights that minimize a distance from $d_i$ under the constraints
    $$\frac{1}{N} \sum_{i \in s} w_i x_i = \frac{1}{N} \sum_{i \in U} x_i \quad \text{and/or} \quad \frac{1}{N} \sum_{i \in s} w_i \hat{\mu}_i = \frac{1}{N} \sum_{i \in U} \hat{\mu}_i.$$
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• Type of model depends on the level of AI available:
  
  – population totals/means → linear models → GREG / calibration
  
  – complete AI → nonlinear/generalized linear/nonparametric models → more general GREG / model calibration
Remote sensed AI in nonparametric model-assisted inference for environmental populations

- Local polynomials GREG on a two-stage sample from the National Resource Inventory Erosion Update Survey (Kim et al., 2004)
- Generalized Additive Models GREG on a two-phase sample from a forest inventory in Utah (Opsomer et al., 2005)
- P-splines GREG to estimate ANC mean for the Northeastern lakes survey (Breidt et al., 2005)
- Neural Networks Model Calibration for streams surveyed in the Mid-Atlantic Highlands (Montanari & Ranalli, 2005)
CDF estimation issues

- Straightforward application of these techniques gives

\[ \hat{F}_G(t) = \frac{1}{N} \sum_{i \in U} \hat{z}_i + \frac{1}{N} \sum_{i \in s} d_i(z_i - \hat{z}_i) \]

with \( \hat{z}_i = I(\hat{\mu}_i \leq t) \).

- Alternatively one can use as the auxiliary variable the estimated probability \( g_i \) of \( y_i \leq t \), i.e.

\[ \hat{F}_G(t) = \frac{1}{N} \sum_{i \in U} g_i + \frac{1}{N} \sum_{i \in s} d_i(z_i - g_i) \]

- This is not a distribution function and can take values outside \([0, 1]\).
CDF estimation: our approach

- We will employ a Nonparametric Model Calibrated Pseudo-Empirical Maximum Likelihood approach
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- Three main pieces of the jigsaw:
  - Nonparametric regression modeling — N — in particular MARS
  - Model Calibration — MC
  - Pseudo-Empirical Maximum Likelihood — PEML
The PEML piece of the jigsaw

The PEML estimator of the CDF is given by

$$\hat{F}_{\text{PEML}}(t) = \sum_{i \in s} \hat{p}_i z_i$$
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with weights such that

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subject to

$$ 0 < p_i < 1, \quad \sum_{i \in s} p_i = 1, \quad \sum_{i \in s} p_i g_i = N^{-1} \sum_{i \in U} g_i $$

where $g_i = g(x_i)$ is a known function of $x_i$ (Chen & Sitter, St.Sinica, 1999).
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where $g_i = g(x_i)$ is a known function of $x_i$ (Chen & Sitter, St.Sinica, 1999).

- Asymptotically equivalent to a GREG if $g(x_i) = x_i$. It looks a lot like calibration!
- (Newton-Raphson type) algorithms to find the solution (Chen et al., Biom.ka, 2002).
- It is equivalent to maximize $l_n(p) = n^* \sum_{i \in s} d_i^* \log p_i$; useful for CI derivation.
The MC piece of the jigsaw – choice of $g_i$'s

For a given value $t_0$ the *optimal* choice (in the sense of Wu, Biometrika, 2003) is

$$g_i = E_\xi(z_i|x_i) = P(y_i \leq t_0|x_i),$$

where $\xi$ is a superpopulation (assisting) model.
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where $\xi$ is a superpopulation (assisting) model.

$\rightarrow$ Given the (binary) nature of the response variable $z_i$, a natural candidate for $\xi$ is the logistic regression model (Chen & Wu, St.Sinica, 2002)

$$\log \left( \frac{g_i}{1 - g_i} \right) = x_i \beta.$$
The N piece of the jigsaw – a more flexible model
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- We therefore extended the logistic model formulation to accommodate non-linear relationships:

$$\log\left(\frac{g_i}{1 - g_i}\right) = \mu(\mathbf{x}_i),$$

where $\mu(\cdot)$ is an unknown function. Nonparametric techniques can be used to obtain (design-based) estimates of $\mu(\cdot)$.

- We will use Multi Adaptive Regression Splines – MARS – in the application.
Confidence intervals

- Instead of using a normal limiting distribution of the estimators, we exploit the pseudo-empirical likelihood nature of the derivation to obtain a CI for $F_N(t)$ at $t = \tilde{t}$. Let’s recall it 9
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• Let $\tilde{p}_i$ be the value of $p_i$ that maximizes $\ln(p)$ subject to

$$0 < p_i < 1, \quad \sum_{i \in s} p_i = 1, \quad \sum_{i \in s} p_i g_i = N^{-1} \sum_{i \in U} g_i, \quad \sum_{i \in s} p_i z_i = \theta,$$

for $z_i = I(y_i \leq \tilde{t})$ and a fixed $\theta$. 
Confidence intervals

• Instead of using a normal limiting distribution of the estimators, we exploit the pseudo-empirical likelihood nature of the derivation to obtain a CI for $F_N(t)$ at $t = \tilde{t}$. Let’s recall it.

• Let $\tilde{p}_i$ be the value of $p_i$ that maximizes $l_n(p)$ subject to

\[
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\]

for $z_i = I(y_i \leq \tilde{t})$ and a fixed $\theta$.

• It can be proved (Wu & Rao, 2004) that the ratio statistics

\[
r_n(\theta) = -2\{l_n(\tilde{p}) - l_n(\hat{p})\} \xrightarrow{d} \chi^2_1,
\]

so that a $(1 - \alpha)$ PEML CI for $F_N(\tilde{t})$ is given by the set

\[
\{\theta | r_n(\theta) < \chi^2_1(\alpha)\}.
\]
Application to ANC CDF estimation in the NE lakes

- Recall that we have \( n = 334 \) possibly averaged measurements of ANC in lakes surveyed from a frame of \( N = 21,026 \).

- The Hajek estimator and the PEML estimator that uses MARS of \( F_N(t) \) have been computed at \( t = (0, 50, 200) \) and at a 1000 value grid.

- The CI computation has been conducted adapting some R functions provided in Wu (WP, 2005).
Modeling issues

- MARS has been used to approximate the unknown function $\mu(x_i)$ in the nonparametric logistic model.

→ Recall the optimal choice of $g_i$: it depends on $t_0 \rightarrow$ no $g_i$ with a fixed $t_0$ can be uniformly optimal for $F_N(t)$ for all values of $t$. 
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→ The model has been fitted at $t_0 = 200$, i.e. the estimated $g_i$ to use in the MCPEML procedure have been obtained only for the model that relates $I(y_i \leq 200)$ to the $x_i$’s and then used for all $t$’s. This is not optimal, but guarantees the achievement of a genuine CDF.
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• The generalized cross validation criterion considered in Friedman (Annals, 1991) suggested the use of 15 basis functions; more interestingly, all variables turned out to be significant according to this criterion: elevation enters as an additive variable (no interactions with other variables), while the $x$ and $y$-geographical coordinates show a significant interaction.
Curves and surfaces estimated by MARS

The vertical axis in each plot shows the contribution of each variable to the whole smooth predictor $\hat{\mu}_i$; since the locations of the plotted functions are arbitrary, they are all translated to have zero minimum value.
CDF estimates at the three thresholds

<table>
<thead>
<tr>
<th></th>
<th>$\hat{F}_H(t)$</th>
<th>95% CI</th>
<th>$\hat{F}_{\text{MARS}}(t)$</th>
<th>95% CI</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.060</td>
<td>(0.017; 0.143)</td>
<td>0.060</td>
<td>(0.017; 0.140)</td>
</tr>
<tr>
<td>50</td>
<td>0.164</td>
<td>(0.104; 0.238)</td>
<td>0.162</td>
<td>(0.103; 0.234)</td>
</tr>
<tr>
<td>200</td>
<td>0.411</td>
<td>(0.301; 0.527)</td>
<td>0.408</td>
<td>(0.311; 0.505)</td>
</tr>
</tbody>
</table>

Cdf estimates at $t = 0, 50, 200$ and relative 95% confidence intervals by the Hajek and Mars estimators. The average length of the confidence intervals is 0.162 with $\hat{F}_H(t)$ and 0.149 with $\hat{F}_{\text{MARS}}(t)$.
CDF estimate and CI bounds at 1000 value grid

The average length of the confidence intervals is 0.209 with \( \hat{F}_H(t) \) and 0.149 with \( \hat{F}_{\text{MARS}}(t) \).
Wrap up

- Nonparametric Model Calibration has been applied to PEML to allow for more flexible models that use complete AI.
- The PEML framework is particularly suitable for CDF estimation: it provides weights with desirable properties and allows for more efficient estimation of confidence bounds.
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- The PEML framework is particularly suitable for CDF estimation: it provides weights with desirable properties and allows for more efficient estimation of confidence bounds.

- An application to ANC CDF estimation in NE lakes has been conducted: the use of AI has shown improvements in estimated efficiency in the form of average confidence bounds 40% wider for the Hajek estimator.

- The application of MARS provides sensible modeling results without unduly *a priori* assumptions on the way the auxiliary variables enter the model.
To do list

- Study the dependance of the final estimates on the choice of the $t_0$ value for which we fit the model and obtain the weights; how much efficiency is lost?
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- Study the dependence of the final estimates on the choice of the $t_0$ value for which we fit the model and obtain the weights; how much efficiency is lost?
- ...then find some sensible guidelines to choose it (!)
- Set up a more thorough simulation study to understand when the PEML CI estimate is better than the simple normal theory one (the PEML one can be *lengthy* for $t$’s faraway from $t_0$).
Essential bibliography and acknowledgments


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