

Modern approaches for component-wise boosting:

Automation, efficiency, and distributed computing with application to the medical domain

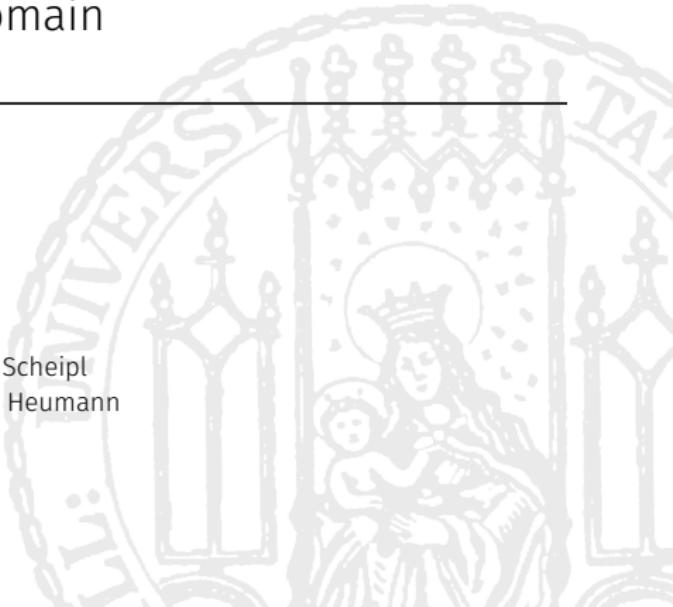
Daniel Schalk

March 24, 2023

Supervisor: Prof. Dr. Bernd Bischl

Referees: Prof. Dr. Matthias Schmid, PD Dr. Fabian Scheipl

Chair of the examination panel: Prof. Dr. Christian Heumann



Overview

Publications

List with all Publications

Structure of the talk

Background

S1

Efficiency

Automation

Distributed computing

Background

Terminology

- p -dimensional covariate or feature vector
 $\mathbf{x} = (x_1, \dots, x_p) \in \mathcal{X} = \mathcal{X}_1 \times \dots \times \mathcal{X}_p$ and target variable $y \in \mathcal{Y}$.
- Data set $\mathcal{D} = \{(\mathbf{x}^{(i)}, y^{(i)}) \mid i = 1, \dots, n\}$ with $(\mathbf{x}^{(i)}, y^{(i)})$ sampled from an unknown probability distribution \mathbb{P}_{xy} .
- True underlying relationship $f : \mathcal{X}^p \rightarrow \mathbb{R}$, $\mathbf{x} \mapsto f(\mathbf{x})$.
- Goal of Machine Learning (ML) is to estimate a model
 $\hat{f} = \arg \min_f \mathcal{R}_{\text{emp}}(f|\mathcal{D})$ with
 - Empirical risk $\mathcal{R}_{\text{emp}}(f|\mathcal{D}) = n^{-1} \sum_{(\mathbf{x}, y) \in \mathcal{D}} L(y, \hat{f}(\mathbf{x}))$ and
 - Loss function $L : \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}_+$, $(y, \hat{y}) \mapsto L(y, \hat{y})$.
- The inducer $\mathcal{I} : \mathbb{D} \times \Lambda \rightarrow \mathcal{F}$, $(\mathcal{D}, \boldsymbol{\lambda}) \mapsto \hat{f} = \mathcal{I}_{\boldsymbol{\lambda}}(\mathcal{D})$ gets a data set $\mathcal{D} \in \mathbb{D}$ with hyperparameters (HPs) $\boldsymbol{\lambda} \in \Lambda$.

Gradient boosting

- Aim is to fit a model \hat{f} by conducting functional gradient descent
$$\hat{f}^{[m-1]} = \hat{f}^{[m]} + \nu \hat{b}^{[m]}.$$
- \hat{b} is a base learner fitted to pseudo residuals
$$r^{[m](i)} = - \left. \frac{\partial L(y^{(i)}, f(x^{(i)}))}{\partial f(x^{(i)})} \right|_{f=\hat{f}^{[m-1]}}, i \in \{1, \dots, n\}$$
- The pseudo residuals contain information in which direction to move $\hat{f}^{[m]}$ for a better fit to the training data \mathcal{D} .
- The fitting is initialized with $\hat{f}^{[0]}(\mathbf{x}) = \arg \min_{c \in \mathcal{Y}} \mathcal{R}_{\text{emp}}(c | \mathcal{D})$ and repeated M times or until an early stopping criterion is met.

Component-wise gradient boosting – Basics

- Compared to GB, component-wise gradient boosting (CWB) can choose from a set of K base learners $b \in \{b_1, \dots, b_K\}$.
- Often, b_1, \dots, b_K are chosen to be (interpretable) statistical models and hence f corresponds to a generalized additive model $f(\mathbf{x}) = f_0 + \sum_{k=1}^K b_k(\mathbf{x})$ with intercept f_0 .
- Advantages of CWB:
 - Feasible to get fit in high-dimensional feature spaces ($p \gg n$).
 - An inherent (unbiased) feature selection.
 - Interpretable/explainable partial feature effects (depending on the choice of base learners).

Component-wise gradient boosting – Algorithm

Algorithm 1 Vanilla CWB algorithm

Input Train data \mathcal{D} , learning rate ν , number of boosting iterations M , loss function L , base learners b_1, \dots, b_K

Output Model $\hat{f} = \hat{f}^{[M]}$

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1: procedure CWB( $\mathcal{D}, \nu, L, b_1, \dots, b_K$ )
2:   Initialize:  $f_0 = \hat{f}^{[0]}(\mathbf{x}) = \arg \min_{c \in \mathcal{Y}} \mathcal{R}_{\text{emp}}(c|\mathcal{D})$ 
3:   while  $m \leq M$  do
4:      $r^{[m]}(i) = - \left. \frac{\partial L(y^{(i)}, f(\mathbf{x}^{(i)}))}{\partial f(\mathbf{x}^{(i)})} \right|_{f=\hat{f}^{[m-1]}}$ ,  $\forall i \in \{1, \dots, n\}$ 
5:     for  $k \in \{1, \dots, K\}$  do
6:        $\hat{\theta}_k^{[m]} = (Z_k^\top Z_k + K_k)^{-1} Z_k^\top r^{[m]}$ 
7:        $\text{SSE}_k = \sum_{i=1}^n (r^{[m]}(i) - b_k(\mathbf{x}^{(i)} | \hat{\theta}_k^{[m]}))^2$ 
8:        $k^{[m]} = \arg \min_{k \in \{1, \dots, K\}} \text{SSE}_k$ 
9:        $\hat{f}^{[m]}(\mathbf{x}) = \hat{f}^{[m-1]}(\mathbf{x}) + \nu b_{k^{[m]}}(\mathbf{x} | \hat{\theta}_{k^{[m]}}^{[m]})$ 
10:    return  $\hat{f} = \hat{f}^{[M]}$ 
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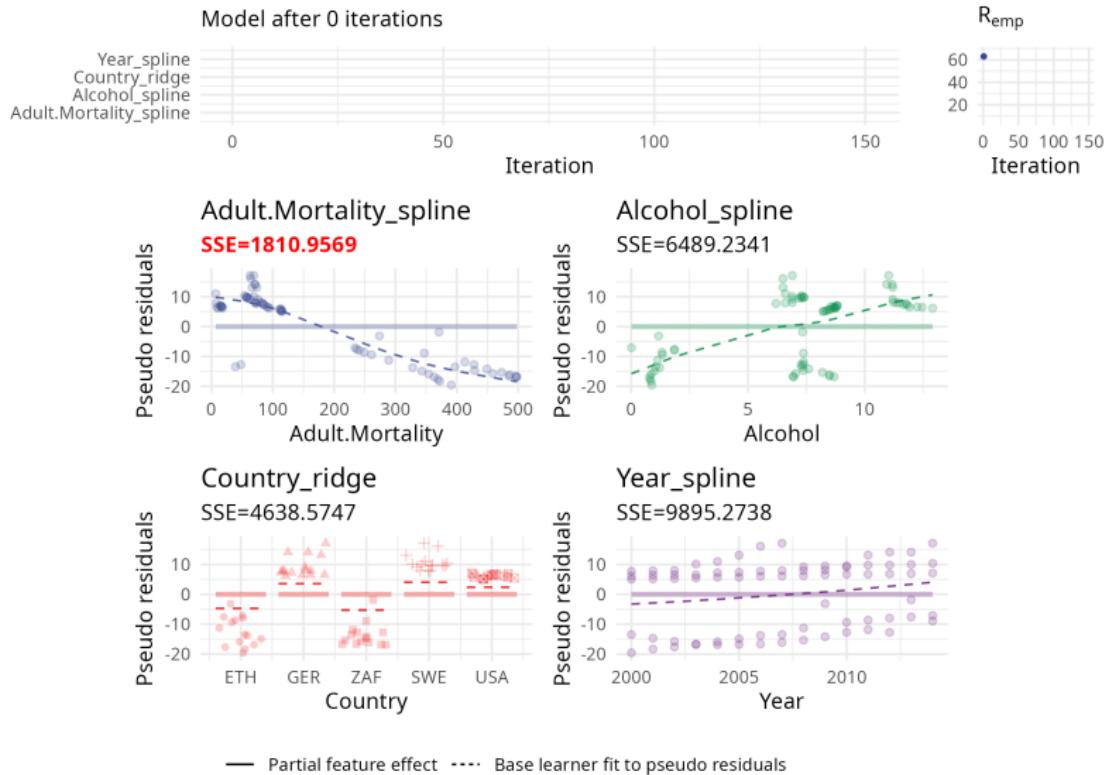
Component-wise gradient boosting – Example

Example throughout this presentation is a subset of a WHO data set¹ about life expectation in years per country:

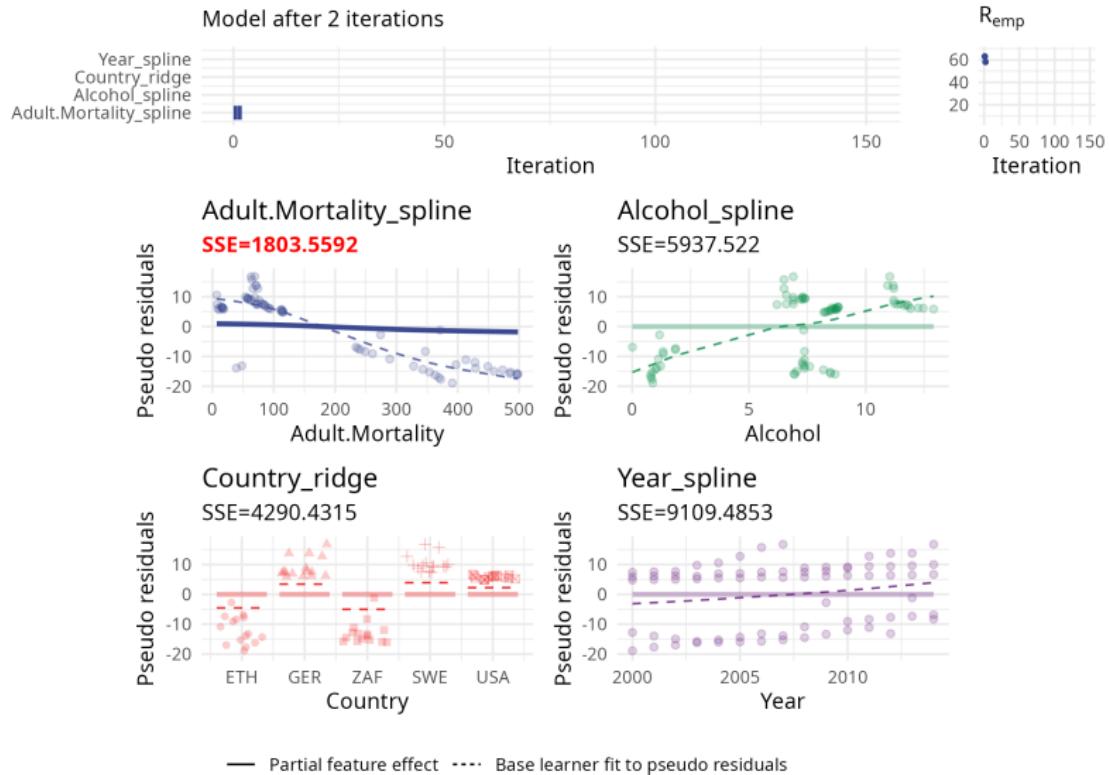
- Target variable is **Life.expectancy** in years.
- Features are **Country**, **Year**, **Alcohol** recorded per capital (15+) consumption (in liters of pure alcohol), and **Adult.Mortality** rates of both sexes of dying between 15 and 60 years per 1000 population.
- Numerical features **Year**, **Alcohol** and **Adult.Mortality** are modeled as P-splines (Eilers and Marx, 1996) and **Country** as one-hot-encoded linear model with ridge penalty.

¹Full description and data is available at
[kaggle.com/datasets/kumarajarshi/life-expectancy-who](https://www.kaggle.com/datasets/kumarajarshi/life-expectancy-who)

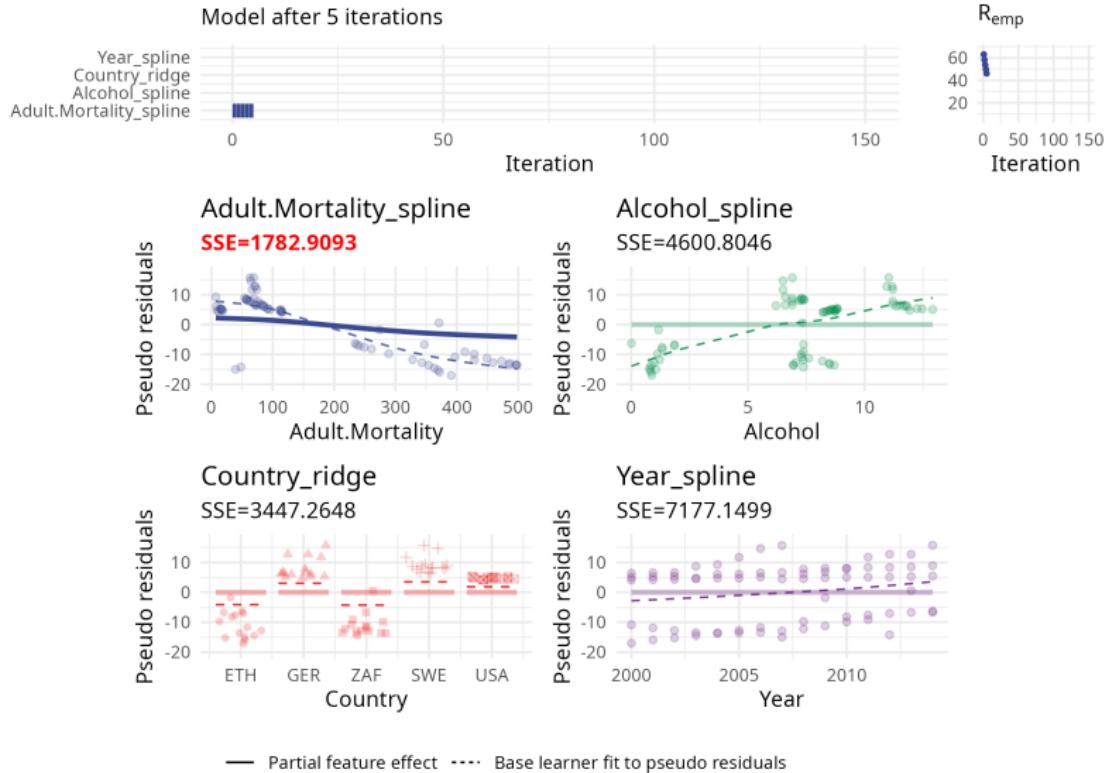
Component-wise gradient boosting – Example



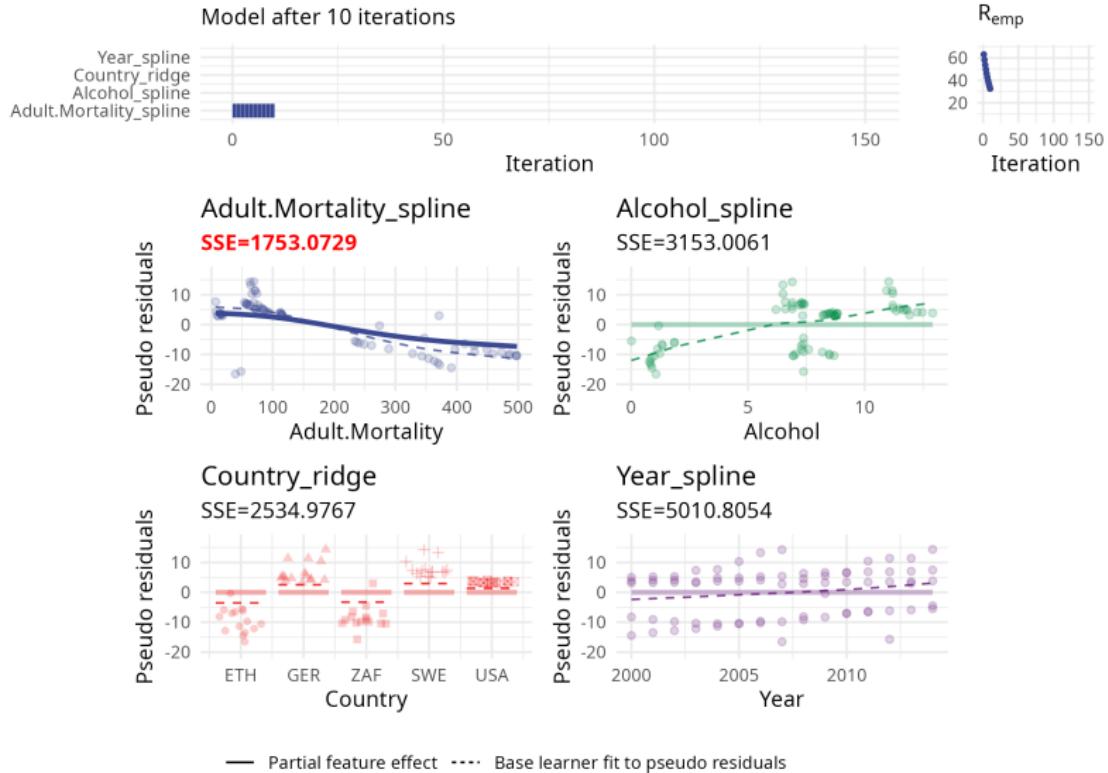
Component-wise gradient boosting – Example



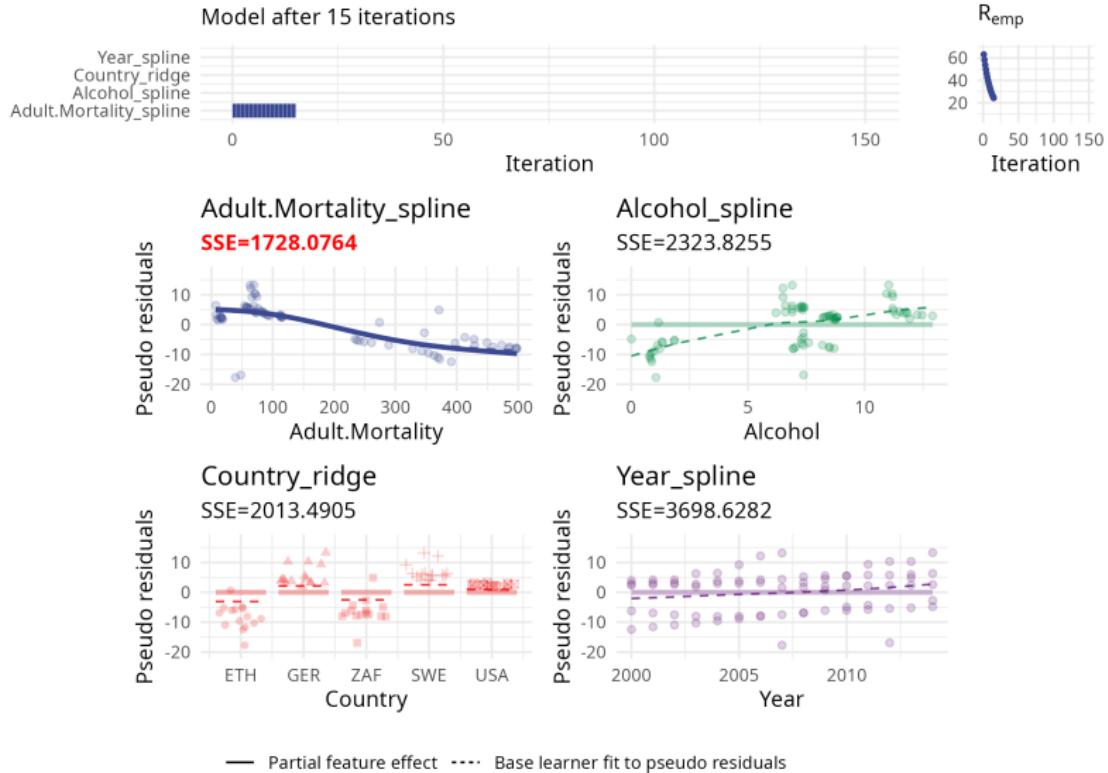
Component-wise gradient boosting – Example



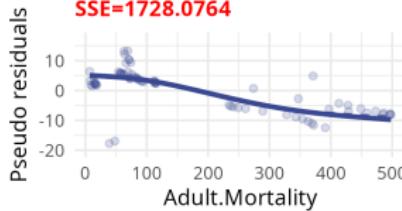
Component-wise gradient boosting – Example



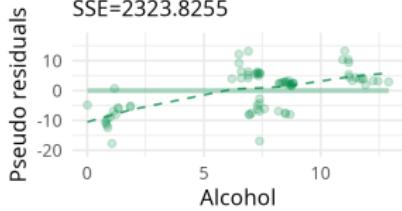
Component-wise gradient boosting – Example



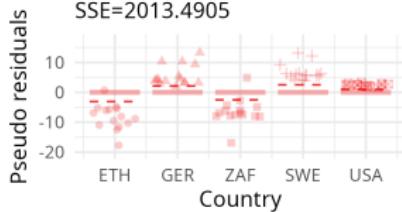
Adult.Mortality_spline
SSE=1728.0764



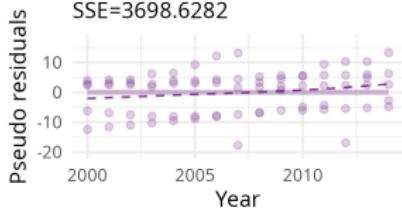
Alcohol_spline
SSE=2323.8255



Country_ridge
SSE=2013.4905

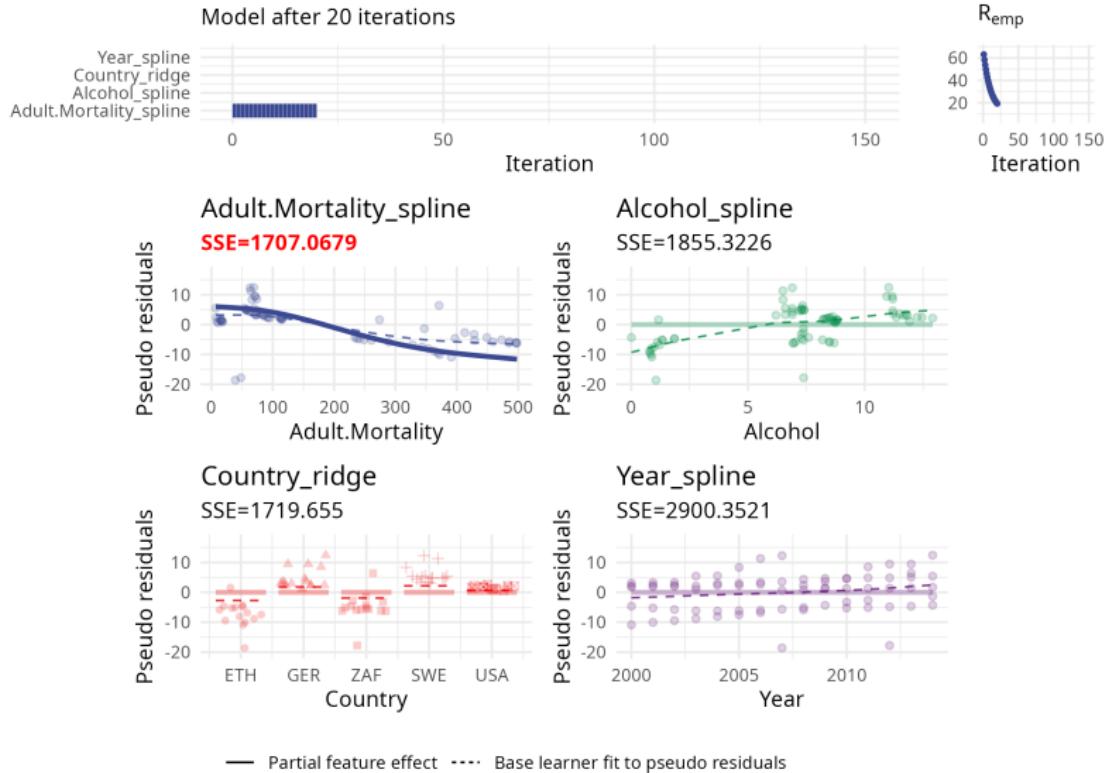


Year_spline
SSE=3698.6282

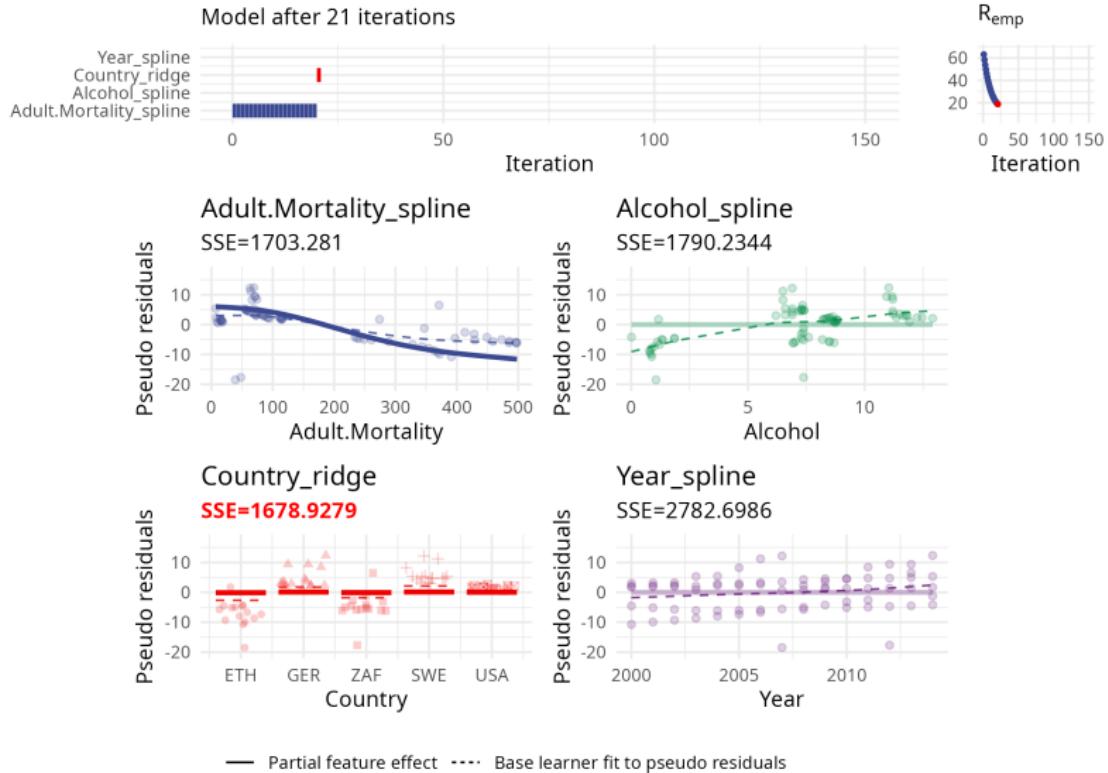


— Partial feature effect ---- Base learner fit to pseudo residuals

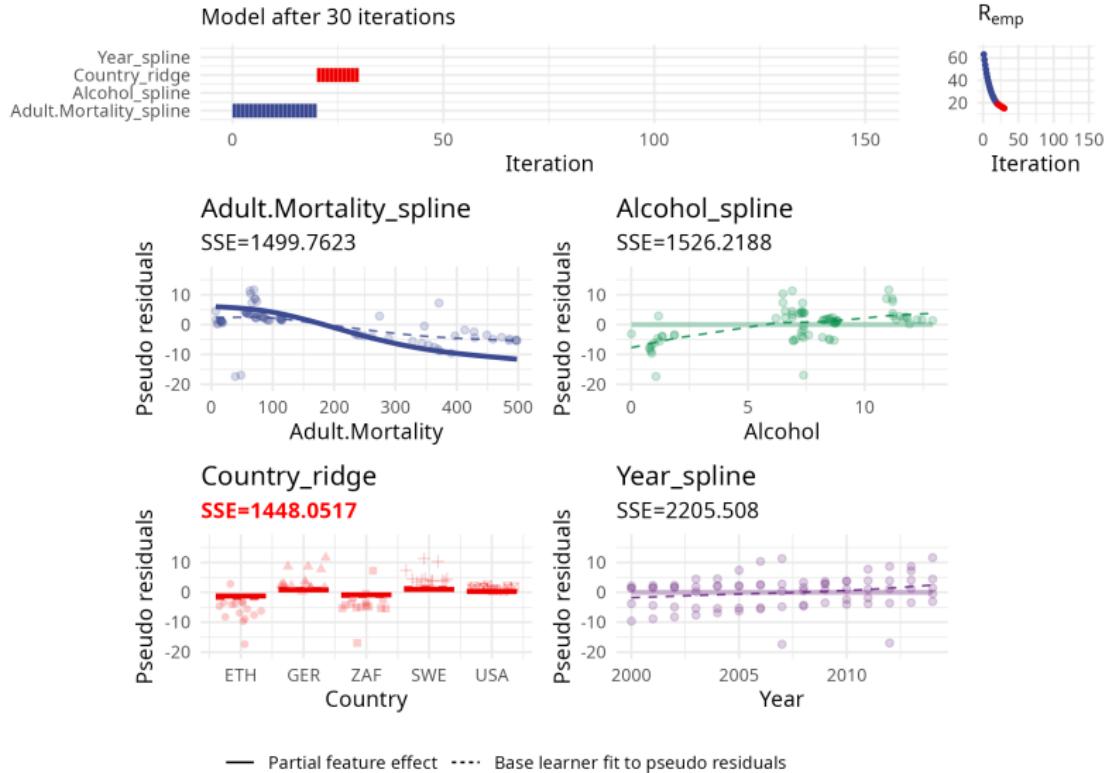
Component-wise gradient boosting – Example



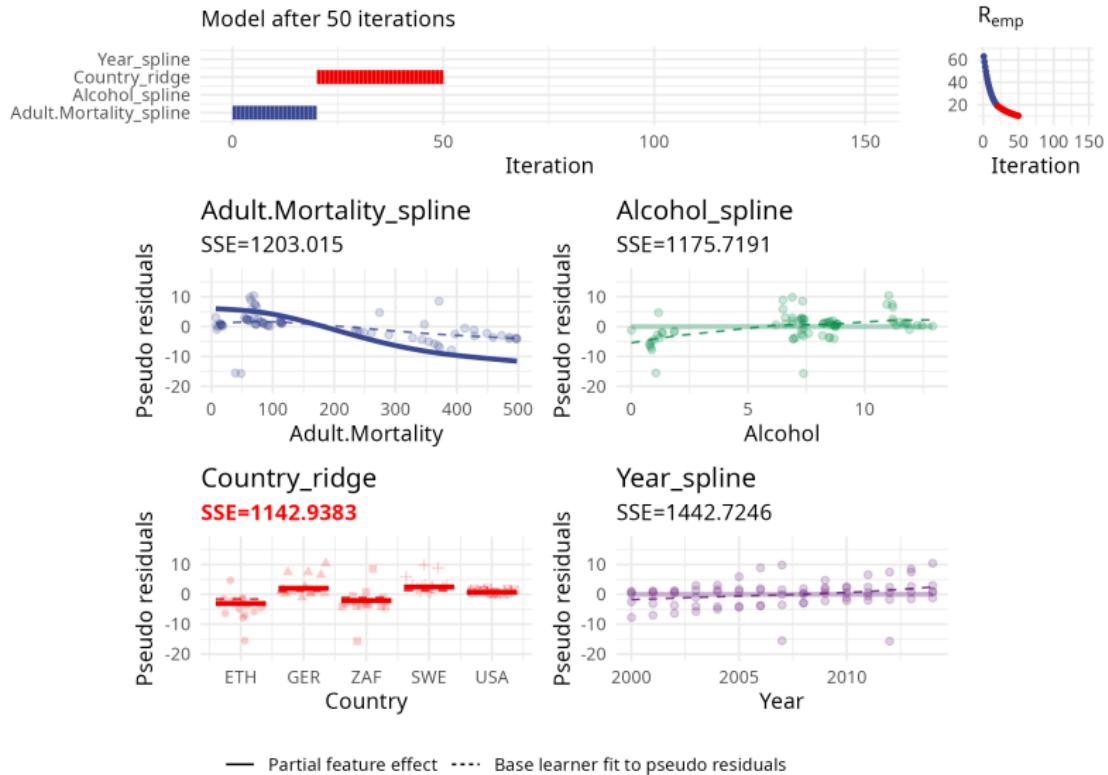
Component-wise gradient boosting – Example



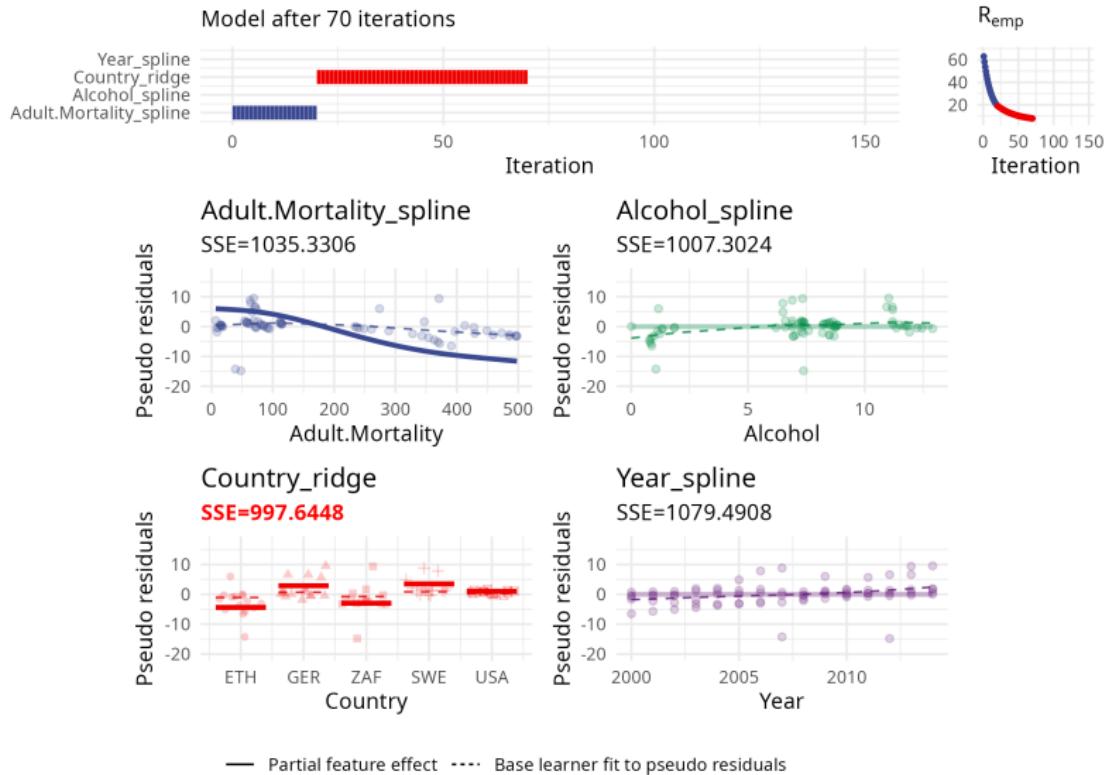
Component-wise gradient boosting – Example



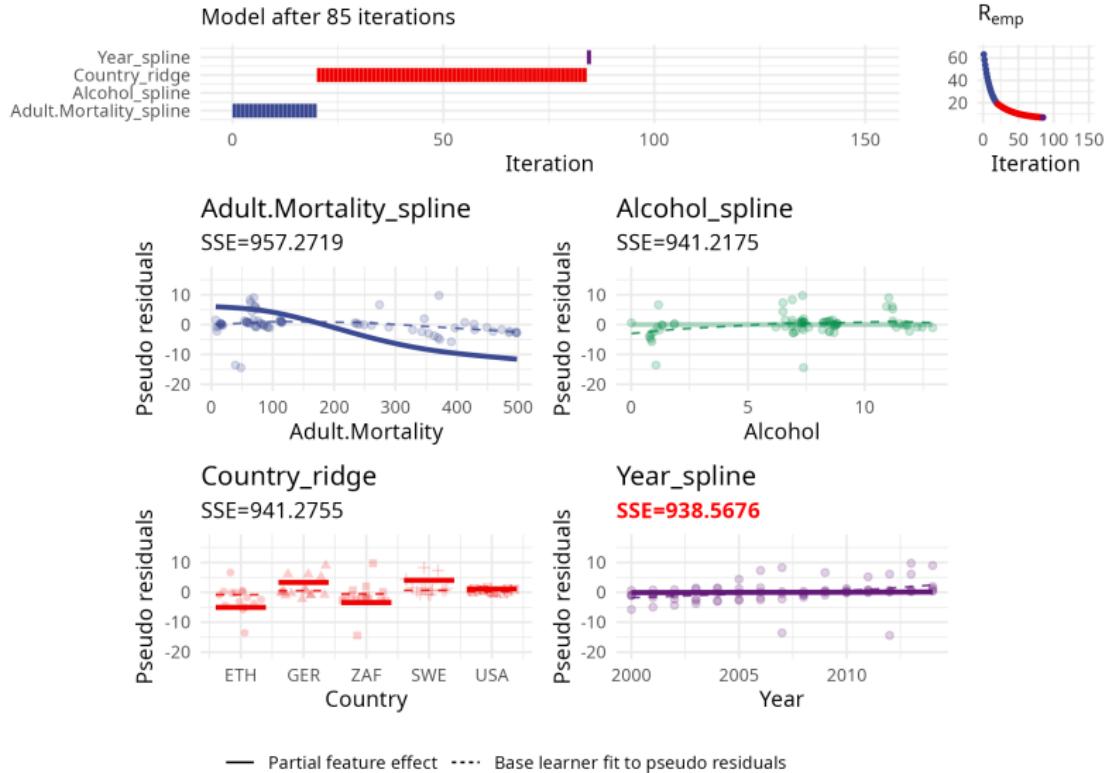
Component-wise gradient boosting – Example



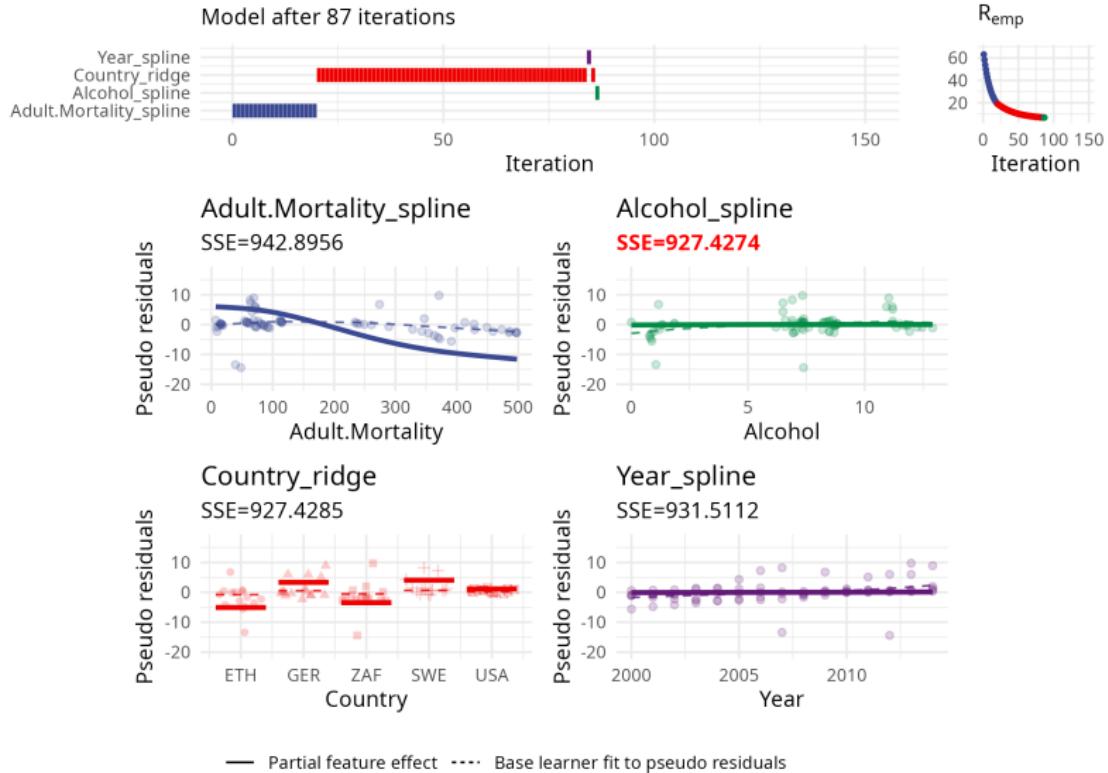
Component-wise gradient boosting – Example



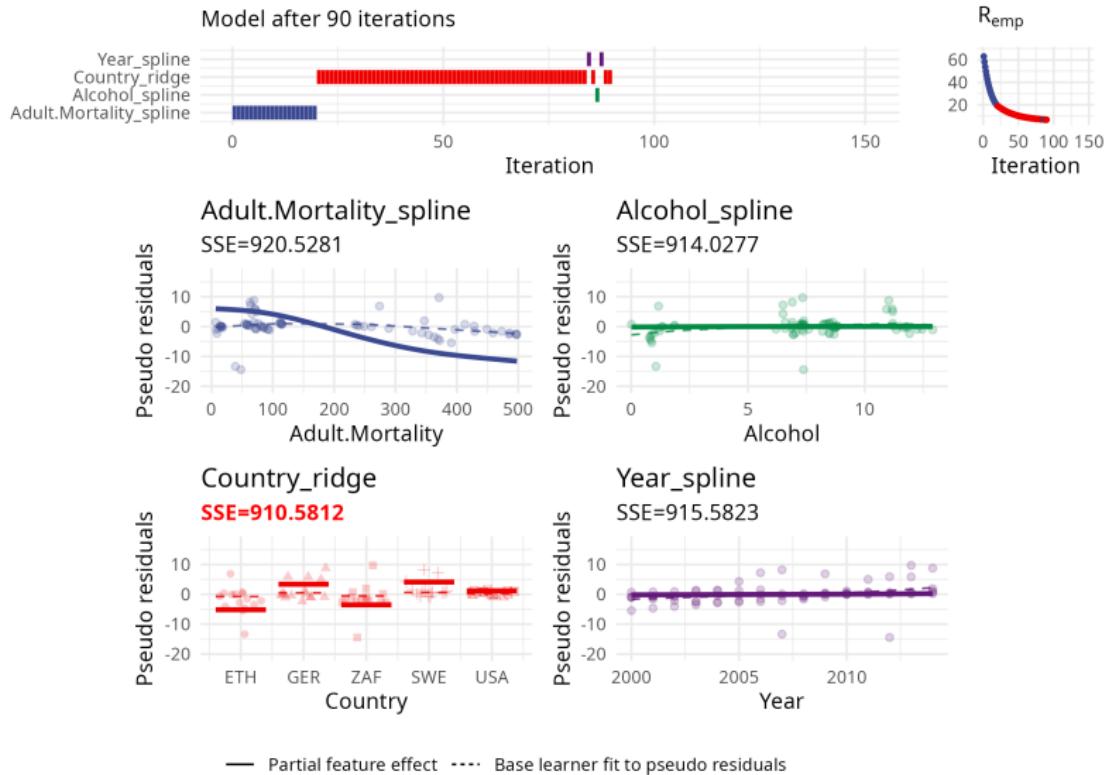
Component-wise gradient boosting – Example



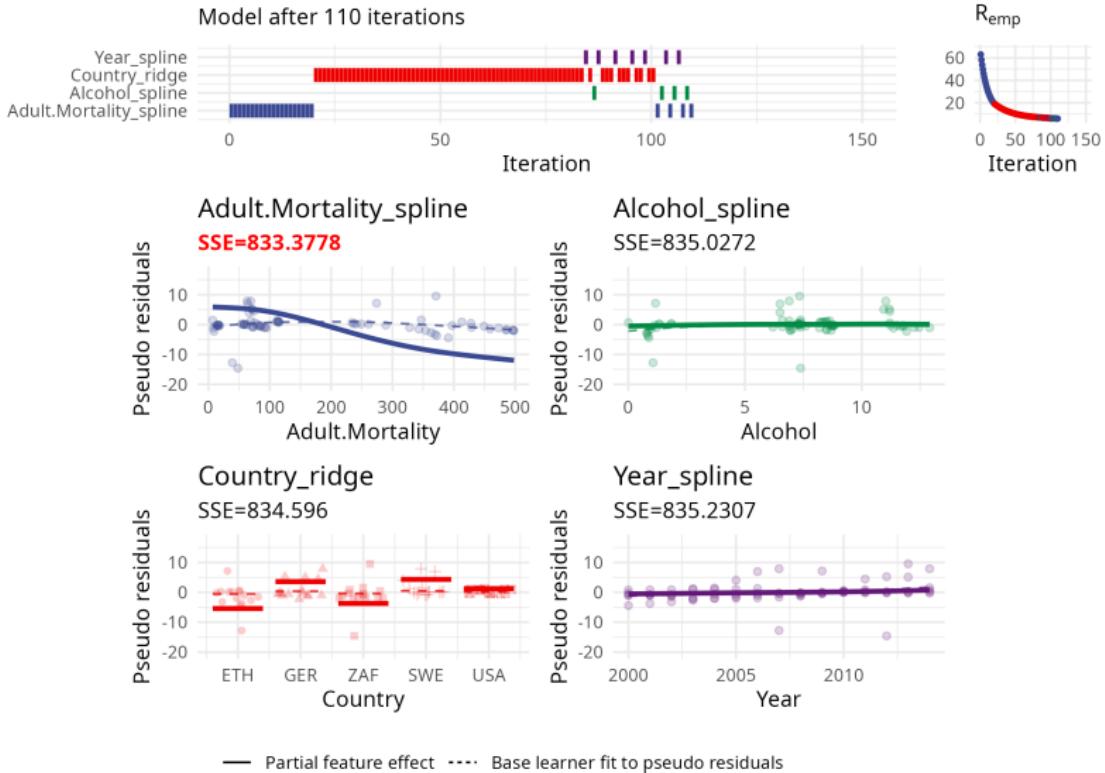
Component-wise gradient boosting – Example



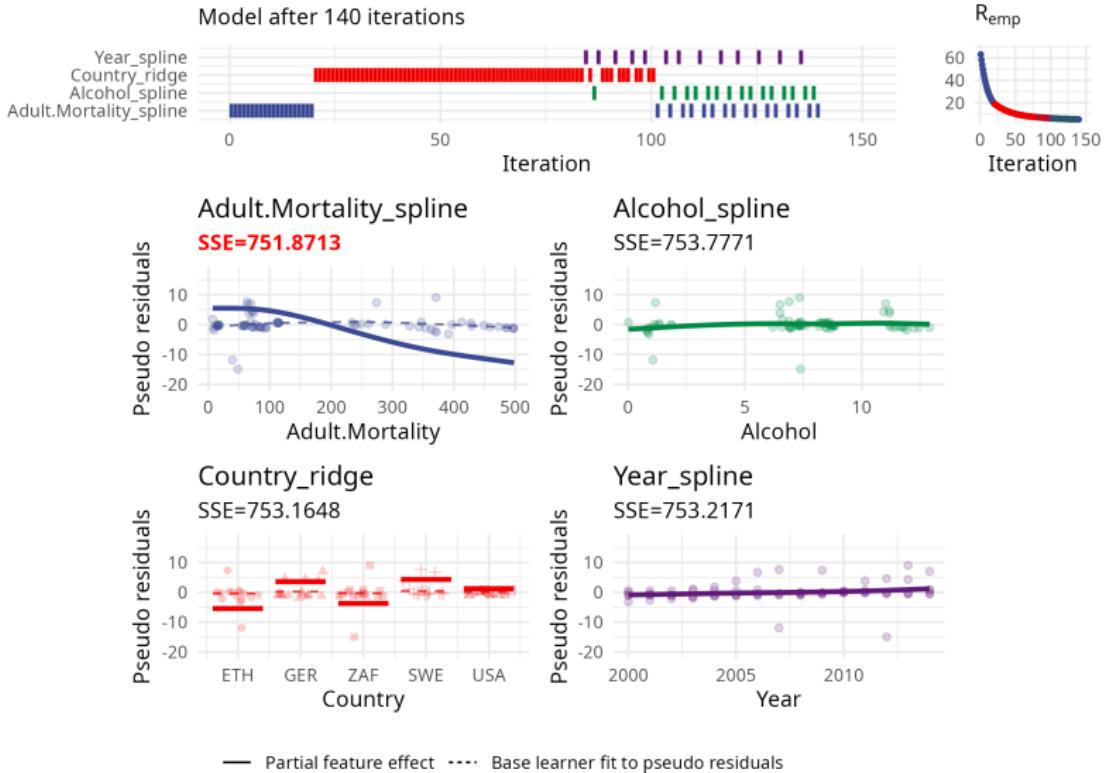
Component-wise gradient boosting – Example



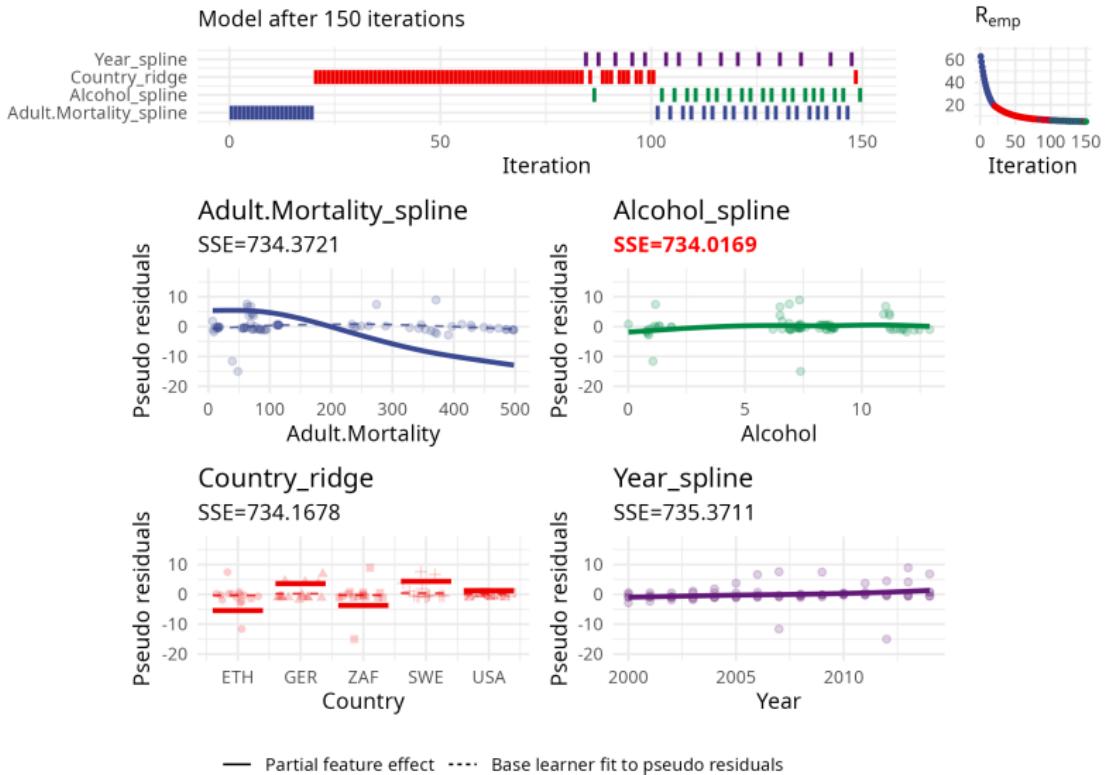
Component-wise gradient boosting – Example



Component-wise gradient boosting – Example



Component-wise gradient boosting – Example



Part I - Efficiency

Name paper here and what it solves

- Memory consumption

Part II - Interpretable ML Framework

Name paper here and what it solves

- Easy access etc.

Part III - Distributed Component-wise Boosting

Name paper here and what it solves

- Distributed etc.

Misc: Distributed Model evaluation, A few slides in the end that describes the issue (sometimes not feasible to just aggregate), how we solved it for the AUC, and what can be done in the future

Efficiency

About

Adaption

About

Results

About

Automation

Automation

About

Autocompboost

About

Results

About

Outlook

About

Distributed computing

Distributed computing

About

Adaption

About

Results

About

Outlook

About

Bla i

Bla (see, e.g., Pepe, 2003), or DeLong et al. (1988)

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