Notes: Generalized Additive Models – Ch4 Introducing GAMs

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Introduction of GAM

- In general the GAM model has a following structure

$$g(\mu_i) = \mathbf{A}_i\boldsymbol{\theta} + f_1(x_{1i}) + f_2(x_{2i}) + f_3(x_{3i}, x_{4i}) + \cdots$$

  - Y_i follows some exponential family distribution: $Y_i \sim EF(\mu_i, \phi)$
  - $\mu_i = E(Y_i)$
  - $\mathbf{A}_i$ is a row of the model matrix, and $\boldsymbol{\theta}$ is the corresponding parameter vector
  - f_j are smooth functions of the covariates x_k

- This chapter
  - Illustrates GAMs by basis expansions, each with a penalty controlling function smoothness
  - Estimates GAMs by penalized regression methods

- **Takeaway: technically GAMs are simply GLM estimated subject to smoothing penalties**

Representing a function with basis expansions

- Let's consider a model containing one function of one covariate

$$y_i = f(x_i) + \epsilon_i, \quad \epsilon_i \overset{\text{iid}}{\sim} \mathsf{N}(0, \sigma^2)$$

- If $b_j(x)$ is the jth basis function, then f is assumed to have a representation

$$f(x) = \sum_{j=1}^{k} b_j(x)\beta_j$$

  with some unknown parameters β_j

  – This is clearly a linear model

The problem with polynomials

- A kth order polynomial is

$$f(x) = \beta_0 + \sum_{j=1}^{k} \beta_k x^k$$

- The polynomial oscillates wildly in places, in order to both interpolate the data and to have all derivatives wrt x continuous

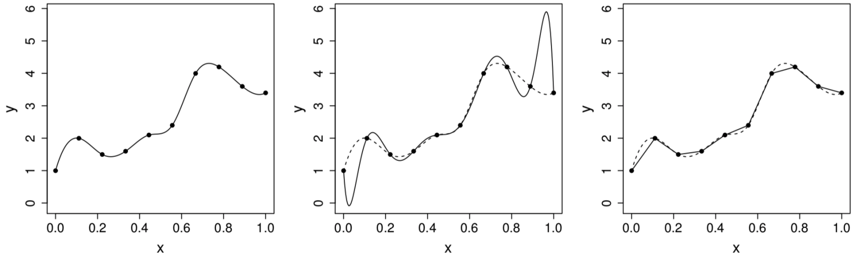


Figure 1: Left: the target function $f(x)$. Middle: polynomial interpolation. Right: piecewise linear interpolant

Piecewise linear basis

- Suppose there are k knots $x_1^* < x_2^* < \cdots < x_k^*$
- The tent function representation of piecewise linear basis is
  - For $j = 2, \ldots, k-1$,

$$b_j(x) = \begin{cases} \frac{x - x_{j-1}^*}{x_j^* - x_{j-1}^*}, & \text{if } x_{j-1}^* < x \leq x_j^* \\ \frac{x_{j+1}^* - x}{x_{j+1}^* - x_j^*}, & \text{if } x_j^* < x \leq x_{j+1}^* \\ 0, & \text{otherwise} \end{cases}$$

  - For the two basis functions on the edge

$$b_1(x) = \begin{cases} \frac{x_2^* - x}{x_2^* - x_1^*}, & \text{if } x \leq x_2^* \\ 0, & \text{otherwise} \end{cases}$$

$$b_k(x) = \begin{cases} \frac{x - x_{k-1}^*}{x_k^* - x_{k-1}^*}, & x > x_{k-1}^* \\ 0, & \text{otherwise} \end{cases}$$

Visualization of tent function basis

- $b_j(x)$ is zero everywhere, except over the interval between the knots immediately to either side of x_j^*
- $b_j(x)$ increases linear from 0 at x_{j-1}^* to 1 at x_j^*, and then decreases linearly to 0 at x_{j+1}^*

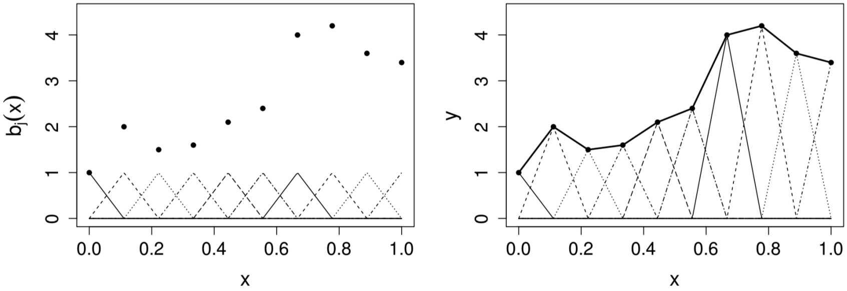


Figure 2: Left: tent function basis, for interpolating the data shown as black dots. Right: the basis functiosn are each multiplied by a coefficient, before being summed

Control smoothness by penalizing wiggliness

- To choose the degree of smoothness, rather than selecting the number of knots k, we can use a relatively large k, but control the model's smoothness by adding a "wiggliness" penalty
  - Note that a model based on $k-1$ evenly spaced knots will not be nested within a model based on k evenly spaced knots
- Penalized likelihood function for piecewise linear basis:

$$\|\mathbf{y} - \mathbf{X}\beta\|^2 + \lambda \sum_{j=2}^{k-1} \left[f(x^*_{j-1}) - 2f(x^*_j) + f(x^*_{j+1}) \right]^2$$

  - Wiggliness is measured as a sum of squared second differences of the function at the knots
  - This crudely approximates the integrated squared second derivative penalty used in cubic spline smoothing
  - λ is called the smoothing parameter

Simplify the penalized likelihood

- For the test function basis, $\beta_j = f(x_j^*)$
- Therefore, the penalty can be expressed as a quadratic form

$$\sum_{j=2}^{k-1} (\beta_{j-1} - 2\beta_j + \beta_{j+1})^2 = \boldsymbol{\beta}^T \mathbf{D}^T \mathbf{D} \boldsymbol{\beta} = \boldsymbol{\beta}^T \mathbf{S} \boldsymbol{\beta}$$

  – The $(k-2) \times k$ matrix $\mathbf{D}$ is

$$\mathbf{D} = \begin{bmatrix} 1 & -2 & 1 & 0 & . & . & . \\ 0 & 1 & -2 & 1 & 0 & . & . \\ 0 & 0 & 1 & -2 & 1 & 0 & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \end{bmatrix}$$

  – $\mathbf{S} = \mathbf{D}^T \mathbf{D}$ is a square matrix

Solution of the penalized regression

- To minimize the penalized likelihood

$$\begin{aligned}\hat{\boldsymbol{\beta}} &= \arg\min_{\boldsymbol{\beta}} \; \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2 + \lambda \boldsymbol{\beta}^T \mathbf{S} \boldsymbol{\beta} \\ &= (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{S})^{-1}\mathbf{X}^T\mathbf{y}\end{aligned}$$

- The hat matrix (also called influence matrix) $\mathbf{A}$ is thus

$$\mathbf{A} = \mathbf{X}(\mathbf{X}^T\mathbf{X} + \lambda\mathbf{S})^{-1}\mathbf{X}^T$$

  and the fitted expectation is $\hat{\boldsymbol{\mu}} = \mathbf{A}\mathbf{y}$

- For practical computation, we can introduce imaginary data to re-formulate the penalized least square problem to be a regular least square problem

$$\|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2 + \lambda \boldsymbol{\beta}^T \mathbf{S} \boldsymbol{\beta} = \left\| \begin{bmatrix} \mathbf{y} \\ \mathbf{0} \end{bmatrix} - \begin{bmatrix} \mathbf{X} \\ \sqrt{\lambda}\mathbf{D} \end{bmatrix} \boldsymbol{\beta} \right\|^2$$

Hyper-parameter tuning

- Between the two hyper-parameters: number of knots k and the smoothing parameter λ, the choice of λ plays the crucial role
- We can always use a k large enough, more flexible then we expect to need to represent $f(x)$
- In `mgcv` package, the default choice is $k = 20$, and knots are evenly spread out over the range of observed data

Choose λ by leave-one-out cross validation

- Under linear regression, to compute leave-one-out cross validation error (called the ordinary cross validation score), we only need to fit the full model once

$$\mathcal{V}_o = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - \hat{f}_i^{[-i]}\right)^2 = \frac{1}{n}\sum_{i=1}^{n}\frac{\left(y_i - \hat{f}_i\right)^2}{(1-A_{ii})^2}$$

  - $\hat{f}_i^{[-i]}$ is the model fitted to all data except y_i
  - $\hat{f}_i$ is the model fitted to all data, and A_{ii} is the ith diagonal entry of the corresponding hat matrix

- In practice, A_{ii} are often replaced by their mean tr$(\mathbf{A})/n$. This results in the generalized cross validation score (GCV)

$$\mathcal{V}_g = \frac{n\sum_{i=1}^{n}\left(y_i - \hat{f}_i\right)^2}{\left[n - \text{tr}(\mathbf{A})\right]^2}$$

From the Bayesian perspective

- The wiggliness penalty can be viewed as a normal prior distribution on β

$$\boldsymbol{\beta} \sim \mathsf{N}\left(\mathbf{0}, \sigma^2 \frac{\mathbf{S}^{-}}{\lambda}\right)$$

  - Because $\mathbf{S}$ is rank deficient, the prior covariance is proportional to the pseudo-inverse $\mathbf{S}^{-}$

- The posterior of β is still normal

$$\boldsymbol{\beta} \mid \mathbf{y} \sim \mathsf{N}\left(\hat{\boldsymbol{\beta}}, (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{S})^{-1}\sigma^2\right)$$

- Given the model this extra structure opens up the possibility of estimating σ^2 and λ using marginal likelihood maximization or REML (aka empirical Bayes)

A simple additive model with two univariate functions

- Let's consider a simple additive model

$$y_i = \alpha + f_1(x_i) + f_2(v_i) + \epsilon_i, \quad \epsilon_i \overset{\text{iid}}{\sim} \mathsf{N}(0, \sigma^2)$$

- The assumption of additive effects is a fairly strong one
- The model now has an identifiability problem: f_1 and f_2 are each only estimable to within an additive constant
  - Due to the identifiability issue, we need to use penalized regression splines

Piecewise linear regression representation

- Basis representation of $f_1()$ and $f_2()$

$$f_1(x) = \sum_{j=1}^{k_1} b_j(x)\delta_j$$

$$f_2(v) = \sum_{j=1}^{k_2} \mathcal{B}_j(v)\gamma_j$$

  – The basis functions $b_j()$ and $\mathcal{B}_j()$ are tent functions, with evenly spaced knots x_j^* and v_j^*, respectively

- Matrix representations

$$\mathbf{f}_1 = [f_1(x_1), \dots, f_1(x_n)]^T = \mathbf{X}_1\boldsymbol{\delta}, \quad [\mathbf{X}_1]_{i,j} = b_j(x_i)$$

$$\mathbf{f}_2 = [f_2(v_1), \dots, f_2(v_n)]^T = \mathbf{X}_2\boldsymbol{\gamma}, \quad [\mathbf{X}_2]_{i,j} = \mathcal{B}_j(x_i)$$

Sum-to-zero constrains to resolve identifiability issues

- We assume
$$\sum_{i=1}^{n} f_1(x_i) = 0 \Longleftrightarrow \mathbf{1}^T \mathbf{f}_1 = 0$$
This is equivalent to $\mathbf{1}^T \mathbf{X}_1 \boldsymbol{\delta} = 0$ for all $\boldsymbol{\delta}$, which implies $\mathbf{1}^T \mathbf{X}_1 = \mathbf{0}$

- To achieve this condition, we can center the column of $\mathbf{X}_1$
$$\tilde{\mathbf{X}}_1 = \mathbf{X}_1 - \mathbf{1}\,\frac{\mathbf{1}^T \mathbf{X}_1}{n}, \quad \tilde{\mathbf{f}}_1 = \tilde{\mathbf{X}}_1 \boldsymbol{\delta}$$

- Column centering reduces the rank of $\tilde{\mathbf{X}}_1$ to $k_1 - 1$, so that only $k_1 - 1$ elements of the k_1 vector $\boldsymbol{\delta}$ can be uniquely estimated

- A simple identifiability constraint:
  - Set a single element of $\boldsymbol{\delta}$ to zero
  - And delete the corresponding column of $\tilde{\mathbf{X}}_1$ and $\mathbf{D}$

- For notation simplicity, in what follows the tildes will be dropped, and we assume that the $\mathbf{X}_j$, $\mathbf{D}_j$ are the constrained versions

Penalized piecewise regression additive model

- We rewrite the penalized regression as

$$\mathbf{y} = \mathbf{X}\beta + \boldsymbol{\epsilon}$$

  where $X = (\mathbf{1}, \mathbf{X}_1, \mathbf{X}_2)$ and $\boldsymbol{\beta}^T = (\alpha, \boldsymbol{\delta}^T, \boldsymbol{\gamma}^T)$

- Wiggliness penalties

$$\boldsymbol{\delta}^T \mathbf{D}_1^T \mathbf{D}_1 \boldsymbol{\delta} = \boldsymbol{\delta}^T \bar{\mathbf{S}}_1 \boldsymbol{\delta} = \boldsymbol{\beta}^T \mathbf{S}_1 \boldsymbol{\beta}, \quad \mathbf{S}_1 = \begin{bmatrix} 0 & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \bar{\mathbf{S}}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{bmatrix}$$

$$\boldsymbol{\gamma}^T \mathbf{D}_2^T \mathbf{D}_2 \boldsymbol{\gamma} = \boldsymbol{\gamma}^T \bar{\mathbf{S}}_2 \boldsymbol{\gamma} = \boldsymbol{\beta}^T \mathbf{S}_2 \boldsymbol{\beta},$$

Fitting additive models by penalized least squares

- Penalized least squares objective function

$$\|\mathbf{y} - \mathbf{X}\beta\|^2 + \lambda_1 \beta^T \mathbf{S}_1 \beta + \lambda_2 \beta^T \mathbf{S}_2 \beta$$

- Coefficient estimator

$$\hat{\beta} = \left(\mathbf{X}^T\mathbf{X} + \lambda_1 \mathbf{S}_1 + \lambda_2 \mathbf{S}_2\right)^{-1} \mathbf{X}^T \mathbf{y}$$

- Hat matrix

$$\mathbf{A} = \mathbf{X}\left(\mathbf{X}^T\mathbf{X} + \lambda_1 \mathbf{S}_1 + \lambda_2 \mathbf{S}_2\right)^{-1} \mathbf{X}^T$$

- Conditional posterior distribution

$$\beta \mid \mathbf{y} \sim \mathsf{N}\left(\hat{\beta}, \hat{\mathbf{V}}_\beta\right), \quad \hat{\mathbf{V}}_\beta = \left(\mathbf{X}^T\mathbf{X} + \lambda_1 \mathbf{S}_1 + \lambda_2 \mathbf{S}_2\right)^{-1} \hat{\sigma}^2$$

Choosing two smoothing parameters

- Since we now have two smoothing parameters λ_1, λ_2, grid searching for the GCV optimal values starts to become inefficient
- Instead, R function `optim` can be used to minimize the GCV score
- We can use log smoothing parameters for optimization to ensure that estimated smoothing parameters are non-negative

Generalized additive models

- Generalized additive models (GAMs): additive models + GLM

$$g(\mu_i) = \alpha + f_1(x_i) + f_2(v_i) + \epsilon_i$$

- Penalized iterative least squares (PIRLS) algorithm: iterate the following steps to convergence

1. Given the current $\hat{\boldsymbol{\eta}}$ and $\hat{\boldsymbol{\mu}}$, compute

$$w_i = \frac{1}{V(\hat{\mu}_i) g'(\hat{\mu}_i)^2}, \quad z_i = g'(\hat{\mu}_i)(y_i - \hat{\mu}_i) + \hat{\eta}_i$$

2. Let $\mathbf{W} = \text{diag}(w_i)$, we obtain the new $\hat{\beta}$ by minimizing

$$\|\sqrt{\mathbf{W}}\mathbf{z} - \sqrt{\mathbf{W}}\mathbf{X}\boldsymbol{\beta}\|^2 + \lambda_1 \boldsymbol{\beta}^T \mathbf{S}_1 \boldsymbol{\beta} + \lambda_2 \boldsymbol{\beta}^T \mathbf{S}_2 \boldsymbol{\beta}$$

Introducing package `mgcv`

- Main function: `gam()`, very much like the `glm()` function
- Smooth terms: `s()` for univariate functions and `te()` for tensors
- A gamma regression example

$$\log\left(E\left[\texttt{Volume}_i\right]\right) = f_1(\texttt{Height}_i) + f_2(\texttt{Girth}_i), \quad \texttt{Volume}_i \sim \text{Gamma}$$

```r
library(mgcv) ## load the package data(trees)
ct1 <- gam(Volume ~ s(Height) + s(Girth),
           family=Gamma(link=log),data=trees)
```

- By default, the degree of smoothness of the f_j is estimated by GCV

```r
summary(ct1)
```

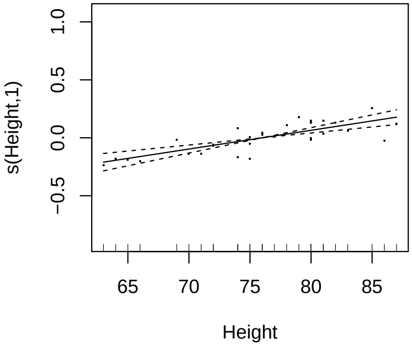
```
##
## Family: Gamma
## Link function: log
##
## Formula:
## Volume ~ s(Height) + s(Girth)
##
## Parametric coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)  3.27570    0.01492   219.6   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Approximate significance of smooth terms:
##             edf Ref.df      F  p-value
## s(Height) 1.000  1.000  31.32 3.92e-06 ***
## s(Girth)  2.422  3.044 219.28  < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## R-sq.(adj) =  0.973   Deviance explained = 97.8%
## GCV = 0.0080824  Scale est. = 0.006899  n = 31
```

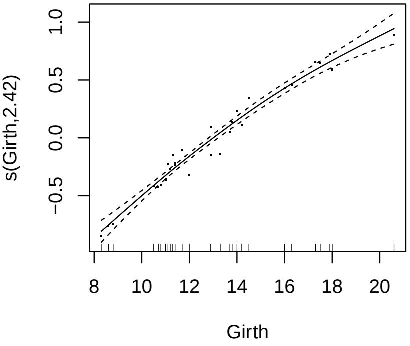
Parital residuals plots

- Pearson residuals added to the estimated smooth terms

$$\hat{\epsilon}_{1i}^{\text{partial}} = f_1(\texttt{Height}_i) + \hat{\epsilon}_i^p$$

```r
par(mfrow = c(1, 2))
plot(ct1,residuals=TRUE)
```





* The number in the y-axis label: effective degrees of freedom

Finer control of `gam()`: choice of basis functions

- Default: thin plat regression splines
  - It has some appealing properties, but can be somewhat computationally costly for large dataset
- We can select penalized cubic regression spline by using

```
s(..., bs = "cr")
```

- We can change the dimension k of the basis
  - The actual effective degrees of freedom for each term is usually estimated from the data by GCV or another smoothness selection criterion
  - The upper bound on this estimate is $k - 1$, minus one due to identifiability constraint on each smooth term

```
s(..., bs = "cr", k = 20)
```

Finer control of `gam()`: the `gamma` parameter

- GCV is known to have some tendency to overfitting
- Inside the `gam()` function, the argument `gamma` can increase the amount of smoothing
  - The default value for `gamma` is 1
  - We can use a higher value to avoid overfitting, `gamma = 1.5`, without compromising model fit

References

- Wood, Simon N. (2017), *Generalized Additive Models: An Introduction with R*. Chapman and Hall/CRC