STAT3612 Lecture 6

Generalized Additive Models

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Generalized Additive Models (GAM)

- Given features $\boldsymbol{x} \in \mathbb{R}^p$, the GAM takes the form

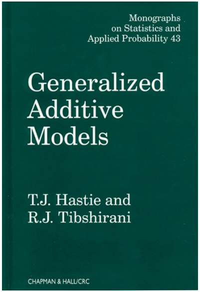
$$g(\mathbb{E}(Y)) = \mu + f_1(x_1) + \cdots + f_p(x_p)$$

  where $g(\cdot)$ is the link function, μ is the overall mean, and $f_j(\cdot)$ is the feature function for x_j.

- $f_j(\cdot)$ can be specified via parametric functions or via feature engineering.

- We consider the nonparametric estimation of $f_j(\cdot)$ subject to certain interpretability constraints.

- GAM dates back to Trevor Hastie and Robert Tibshirani (1990). See also Wikipedia.



Backfitting Algorithm

In statistics, the backfitting algorithm is a particularly useful procedure for fitting GAMs iteratively. See Wikipedia for details. It provides a greedy sub-optimal solution though.

For regression case with $g(y) = y$, the backfitting algorithm is as simple as

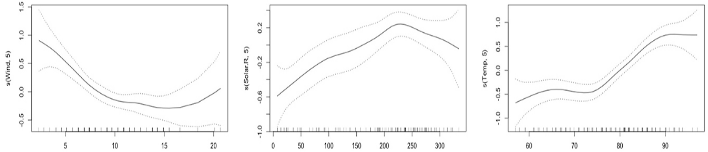
1. Initialize $\bar{\mu} = \bar{y}$ and $\hat{f}_j \equiv 0 \; \forall j$
2. Cycle through $j = 1, \ldots, p$, perform univariate smoothing

$$\hat{f}_j(x_{ij} \leftarrow S_j\left(\left\{y_i - \hat{\mu} - \sum_{k \neq j} \hat{f}_k(x_{ik})\right\}_{i=1}^{n}\right)$$

   where $S_j(\cdot)$ is a smoothing operator to be discussed in this chapter.

3. Continue Step 2 until the individual functions do not change.

Feature Representation by Nonparametric Smoothing



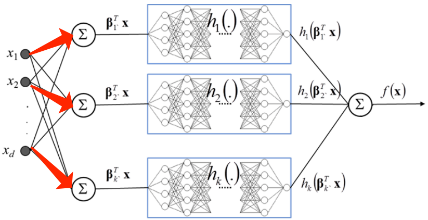
Each univariate $f_j(x_j)$ in a GAM is data-driven, subject to the following interpretability constraints:

- **Homogeneously Smooth:** classical nonparametric regression
  $\Rightarrow$ Kernel/Scatterplot smoothing: loess, local linear regression
  $\Rightarrow$ Smoothing splines, Hodrick-Prescott filter (ℓ_2-penalty)
- **Inhomogeneously Smooth:** e.g. piecewise-constant, piecewise-linear
  $\Rightarrow$ ℓ_1/ℓ_0-trend filtering with automatic knot detection
  $\Rightarrow$ $\ell_2/\ell_1/\ell_0$-penalized B-Splines
- **Shape Constraints:** e.g. increasing/decreasing, convex/concave
  $\Rightarrow$ Monotone/Isotonic regression, Least concave majorant

GAM for Interpretable Machine Learning

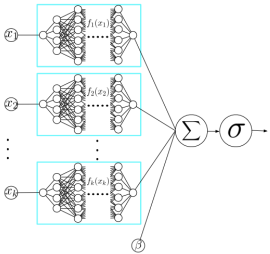
- The classical GAM (Hastie and Tibshirani, 1990) provides an important class of interpretable machine learning today.
- It can take advantages of deep learning for automated sub-modular feature representation, resulting in optimized solution via SGD network training.

GAM-Net (Special case of xNN)



Vaughan, Sudjianto, Brahimi, Chen, and Nair (2018)
Yang, Zhang and Sudjianto (2019)

NAM (Neural Additive Model)



Agarwal, Frosst, Zhang, Caruana, and Hinton (2020)

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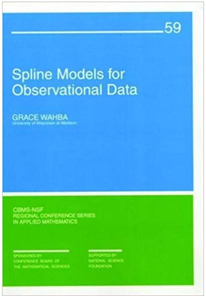
Smoothing Spline



Grace Wabha: Spline Models for Observational Data (1990)

Smoothing Spline

- Smoothing spline is a basic tool for nonparametric regression. It controls the degree of smoothness through the roughness penalty:

$$\min_{f \in \mathcal{H}} \sum_{i=1}^{n} [y_i - f(x)]^2 + \lambda \int |f''(u)|^2 du$$

  where $\mathcal{H}$ denotes the 2nd-order Sobolev space.

- When $\lambda = 0$, there is no smoothing effect, but only interpolating.

- When $\lambda = \infty$, $|f''(x)| = 0$ for all x, which results in a line.

B-Spline Representation

- The unique minimizer is a cubic spline with knots at the unique x_i.
- By expressing $f(x) = \boldsymbol{\beta}^T \boldsymbol{\phi}(x)$ through use of B-spline bases, we can solve

$$\min_{\boldsymbol{\beta}} (\mathbf{y} - \boldsymbol{\Phi}\boldsymbol{\beta})^T (\mathbf{y} - \boldsymbol{\Phi}\boldsymbol{\beta}) + \lambda \boldsymbol{\beta}^T \boldsymbol{\Omega} \boldsymbol{\beta}$$

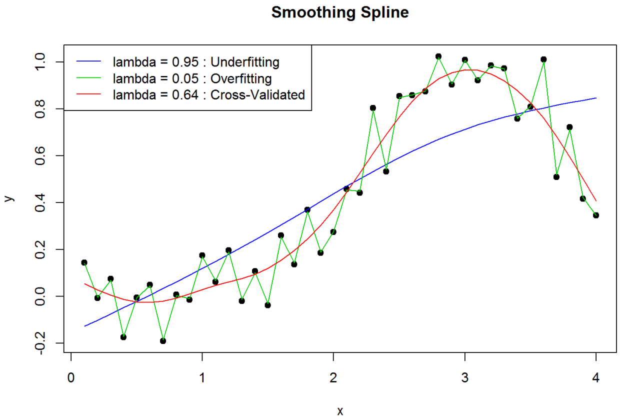
  where $\Omega_{ij} = \int \ddot{\phi}_i(x) \ddot{\phi}_j(x) dx$. It leads to the generalized ridge estimator:

$$\hat{\boldsymbol{\beta}}_\lambda = (\boldsymbol{\Phi}^T \boldsymbol{\Phi} + \lambda \boldsymbol{\Omega})^{-1} \boldsymbol{\Phi}^T \mathbf{y}$$

- The smooth curve is given by $\hat{\boldsymbol{y}} = \mathbf{S}_\lambda \mathbf{y}$, where the smoothing matrix is

$$\mathbf{S}_\lambda = \boldsymbol{\Phi}(\boldsymbol{\Phi}^T \boldsymbol{\Phi} + \lambda \boldsymbol{\Omega})^{-1} \boldsymbol{\Phi}^T$$

Smoothing Spline Fits

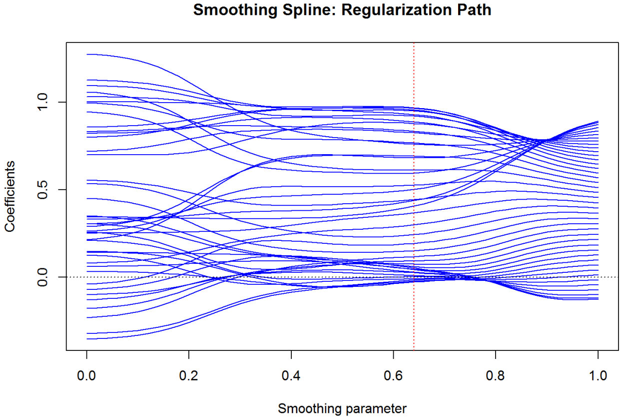


Regularization Paths

R code:

```
ss = seq(0, 1, by=0.02)
bb = NULL
for (k in 1:length(ss)) {
  tmp = smooth.spline(x, y, spar=ss[k])
  bb = cbind(bb, tmp$fit$coef)
}
matplot(ss, t(bb), type='l', lty=1, lwd = 1, col=4,
        xlab = "Smoothing parameter", ylab = "Coefficients",
        main = 'Smoothing Spline: Regularization Path')
abline(v= smooth.spline(x, y, cv = TRUE)$spar, col=2, lty=3,lwd=1)
abline(h=0, lty=3, col=1)
```

Regularization Paths



Cross-Validation

1. Split the re-shuffled data into K (e.g. 5, 10, n) folds
2. For each fold $k = 1, \ldots, K$:
   - Fit model based on the remaining K-1 folds of data
   - Evaluate the fitted model on the left-out fold
3. Take the average risk (i.e. MSE) as the cross-validation score

Cross-Validation

- Smoothing spline usually adopts the **GCV** (generalized cross-validation) based on the leave-one-out scheme (i.e. n-fold).

- For $i = 1, \ldots, n$, let $\hat{f}^{[i]}(x_i)$ denote the prediction at x_i based on the leave-one-out sample $\{(x_j, y_j)\}_{j \neq i}$, define

$$\mathrm{LOOCV}(\lambda) = \frac{1}{n} \sum_{i=1}^{n} \left(y_i - \hat{f}^{[i]}(x_i) \right)^2$$

- Upon some relaxation, the LOOCV score can be approximated by the following GCV score:

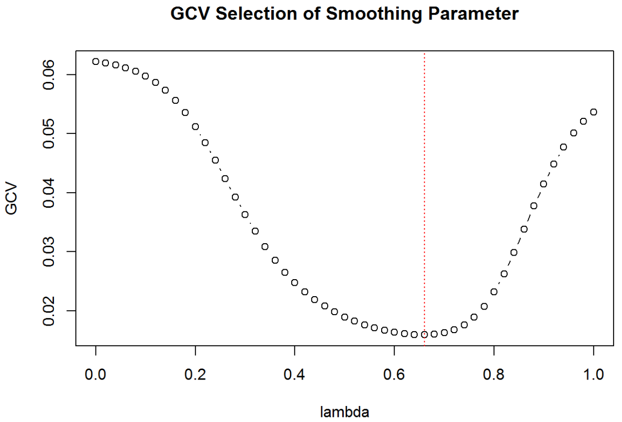
$$\mathrm{GCV}(\lambda) = \frac{1}{n} \sum_{i=1}^{n} \left(\frac{y_i - \hat{f}(x_i)}{1 - \mathrm{tr}(\mathbf{S}_\lambda)/n} \right)^2$$

Cross-Validation

R code:

```
ss = seq(0, 1, by=0.02)
gcv = NULL
for (k in 1:length(ss)) {
  tmp = smooth.spline(x, y, spar=ss[k])
  gcv = c(gcv, tmp$cv.crit)
}
plot(ss, gcv, type='b',
     xlab="lambda", ylab="GCV",
     main="GCV Selection of Smoothing Parameter")
abline(v=ss[which.min(gcv)],col=2,lty=3,lwd=1)
```

Cross-Validation



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HP Trend Filtering

- Let $\{y_i\}_{i\in[n]}$ be the sequence data observed regularly (with equal spacing).
- Assume $y_i = \alpha_i + \varepsilon_i$, with α_i representing the underlying signal/trend.
- HP ℓ_2-trend filtering by Hodrick and Prescott (1997):

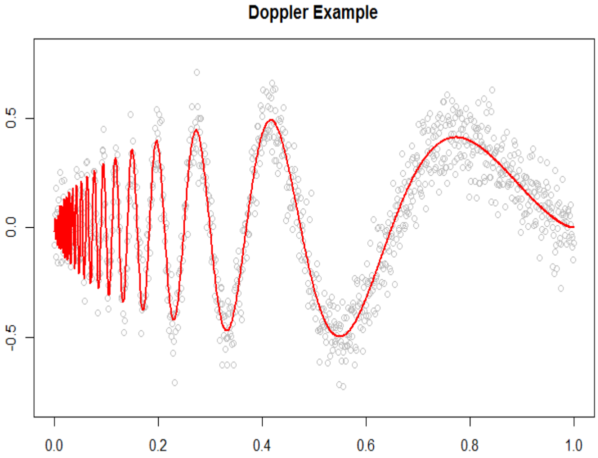
$$\min_{\{\alpha_i\}} \frac{1}{2}\sum_{i=1}^{n}(y_i - \alpha_i)^2 + \lambda \sum_{i=2}^{n-1}(\alpha_{i-1} - 2\alpha_i + \alpha_{i+1})^2$$

- It can be viewed as the smoothing spline under the discrete setting:

$$\min_{\boldsymbol{\alpha}\in\mathbb{R}^n} \frac{1}{2}\|\boldsymbol{y} - \boldsymbol{\alpha}\|_2^2 + \lambda\|\boldsymbol{D}^{(2)}\boldsymbol{\alpha}\|_{\ell_2}^2,$$

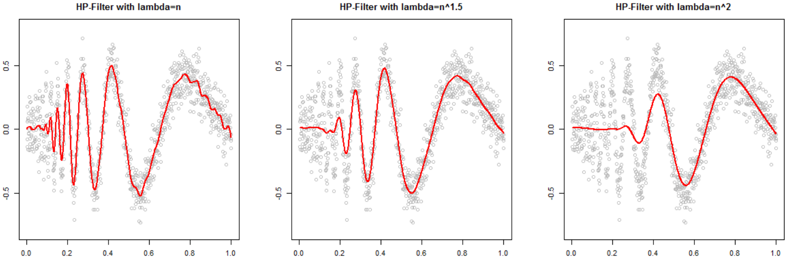
- $\boldsymbol{D}^{(2)} = [\cdots;0\ldots0,1,-2,1,0\ldots0;\cdots]$ is the 2nd-order difference matrix

Illustrative Examples



R:hpfilter Results

- R package: https://cran.r-project.org/package=mFilter
- Use `hpfilter(y, type="lambda", freq)` with λ-specification



Trend Filtering: ℓ_1 approach

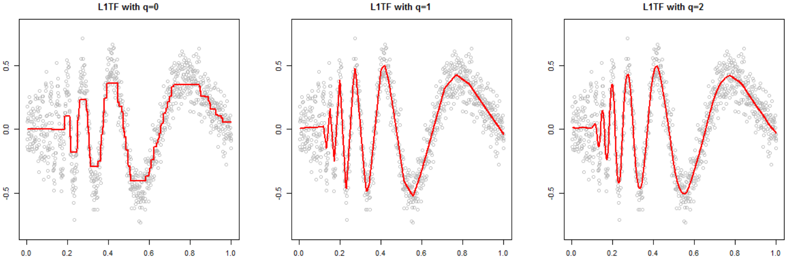
- ℓ_1-trend filtering by Kim, et al. (2009) and Tibshiran (2014):

$$\min_{\boldsymbol{\alpha} \in \mathbb{R}^n} \frac{1}{2} \|\boldsymbol{y} - \boldsymbol{\alpha}\|_2^2 + \lambda \|\boldsymbol{D}^{(q+1)} \boldsymbol{\alpha}\|_{\ell_1}, \quad q = 0, 1, 2, \ldots$$

- Extended to different orders of finite differences.
- The ℓ_1-penalty induces the piecewise smoothness.
- Hyperparameter can be determined by the BIC criterion.

ℓ_1-Trend Filtering Results

- R package at https://github.com/glmgen/glmgen
- Use `trendfilter(y, k=q)` plus BIC parameter tuning



Research on ℓ_0-Trend Filtering

- The ℓ_0-regularized trend filtering problem is formulated by

$$\min_{\boldsymbol{\alpha} \in \mathbb{R}^n} \frac{1}{2}\|\boldsymbol{y} - \boldsymbol{\alpha}\|_2^2 + \lambda\|\boldsymbol{D}^{(q+1)}\boldsymbol{\alpha}\|_{\ell_0}, \quad q = 0, 1, 2, \ldots$$

- Much more promising results, but challenging with ℓ_0-optimization
- R:AMIAS Package: https://cran.r-project.org/package=AMIAS

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Penalzied B-Splines

- Initialize B-Spline bases (degree q) with dense knots (equal spaced)
- Run the ℓ_2-penalized regression:

$$\min_{\boldsymbol{\alpha} \in \mathbb{R}^n} \frac{1}{2} \|\boldsymbol{y} - \boldsymbol{\Phi}\boldsymbol{\alpha}\|_2^2 + \lambda \|\boldsymbol{D}^{(q+1)}\boldsymbol{\alpha}\|_{\ell_2}^2,$$

  where $\boldsymbol{\Phi}$ represents the design matrix generated by B-Spline bases.

- It leads to the closed-form solution (generalized ridge estimator):

$$\hat{\boldsymbol{y}} = \boldsymbol{\Phi}\left(\boldsymbol{\Phi}^T \boldsymbol{\Phi} + \lambda (\boldsymbol{D}^{(q+1)})^T \boldsymbol{D}^{(q+1)}\right)^{-1} \boldsymbol{\Phi}^T \boldsymbol{y}$$

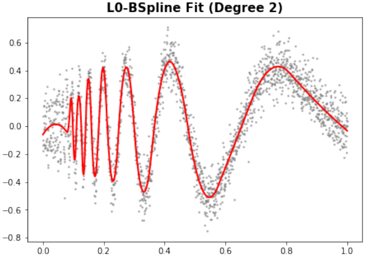
- Note that this is used by the pyGAM package (to be discussed).

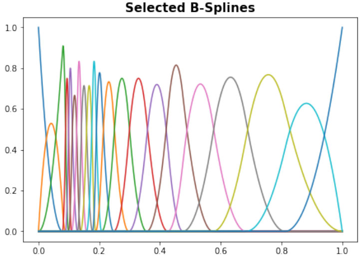
Research on ℓ_0-penalized B-Splines

- Ongoing investigation by switching ℓ_2-penalty to ℓ_0-penalty:

$$\min_{\boldsymbol{\alpha} \in \mathbb{R}^n} \frac{1}{2} \|\boldsymbol{y} - \boldsymbol{\Phi}\boldsymbol{\alpha}\|_2^2 + \lambda \|\boldsymbol{D}^{(q+1)}\boldsymbol{\alpha}\|_{\ell_0},$$

- An iterative reweighing solution being developed, with promising results:





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The pyGAM Package

- A Python package for GAM: https://github.com/dswah/pyGAM
- `pip install pygam`
- The pyGAM package adopts the ℓ_2-penalized B-splines.
- It supports increasing/decreasing, convex/concave constraints.
- It comes with "partial dependency plot" for visualizing feature functions.
- See the supplementary Python code/notebook for demonstration with examples ...

Thank You!

Q&A or Email ajzhang@umich.edu