Advanced Statistical Modeling

Part 2. Nonparametric Modeling

Session 7: Generalized additive models and Semiparametric models

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Multiple nonparametric regression

- The extension of the nonparametric regression model to the case in which there are p explanatory variables is straightforward:

$$y_i = m(x_{i1}, \dots, x_{ip}) + \varepsilon_i,$$

  with $E(\varepsilon_i) = 0$ and $V(\varepsilon_i) = \sigma^2$, for $i = 1, \dots, n$.
- The regression function m indicates how y varies depending on the p-dimensional explanatory variable $\mathbf{x} = (x_1, \dots, x_p)$.
- To define the local polynomial estimator of the regression function $m(\mathbf{x})$ we need, first, to define the weights w_i for each observation, and secondly, to specify which explanatory variables are included at each local linear regression model.

Defining the weights w_i

- When estimating $m(\mathbf{t})$, with $\mathbf{t} = (t_1, \dots, t_p)$, data $(y_i; x_{i1}, \dots, x_{ip})$ with $\mathbf{x_i} = (x_{i1}, \dots, x_{ip})$ closer to $\mathbf{t} = (t_1, \dots, t_p)$ should have greater weight than those data that are further.
- Now distances between $\mathbf{t}$ and $\mathbf{x_i}$ are measured in a p-dimensional space and there are many sensible ways to define distances in such space.
- A way to define weights w_i with good performance in practice is

$$w_i = w(\mathbf{t}, \mathbf{x}_i) \propto \prod_{j=1}^{p} K\left(\frac{x_{ij} - t_j}{h_j}\right),$$

where K is a univariate kernel function, h_j is a smoothing parameter well suited for variable j-th, and symbol $\propto$ means proportionality.

Explanatory variables at each local linear model

- To fit a degree q polynomial depending on p-variables, all possible terms with the form

$$\beta_{s_1 \cdots s_p} \prod_{j=1}^{p} (x_{ij} - t_j)^{s_j},$$

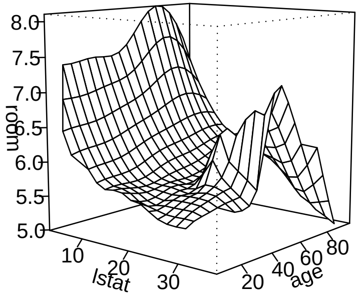
with degree $\sum_{j=1}^{p} s_j \leq q$, must be included.
- The estimate of $m(\mathbf{t})$ will be the intercept of the local polynomial fitted around point $\mathbf{t}$: $\hat{m}(\mathbf{t}) = \hat{m}(t_1, \ldots, t_p) = \hat{\beta}_{0\ldots0}$.
- Example. Two explanatory variables, local polynomial with degree 2,

$$\beta_{00} + \beta_{10}(x_{i1} - t_1) + \beta_{01}(x_{i2} - t_2) + \beta_{11}(x_{i1} - t_1)(x_{i2} - t_2) + \beta_{20}(x_{i1} - t_1)^2 + \beta_{02}(x_{i2} - t_2)^2.$$

The estimate of m at $\mathbf{t} = (t_1, t_2)$ will be $\hat{\beta}_{00}$.

Example: Boston housing data, bivariate regression.

- Nonparametric fit of `ROOM` as a function of `LSTAT` and `AGE`.
- `AGE`: For each neighborhood, the percentage of houses built before 1940.
- A kernel product of two univariate Gaussian kernels is used.
- Smoothing parameters: $h_1 = 2.5$ for `LSTAT`, and $h_2 = 10$ for `AGE`.



Practice:

Bivariate non-parametric regression with library **sm**

The curse of dimensionality

- A general problem in multivariate nonparametric estimation, and in particular in nonparametric regression with multiple regressors, is the phenomenon known as curse of dimensionality:

  In high dimensional spaces the neighborhood of any point $\mathbf{t}$ contains virtually no observational data.

- To construct a ball centered at a point $\mathbf{x_0} \in \mathbb{R}^d$ that contains say the 25% of the observed points, the ball must be so large that we can hardly say that it represents a neighborhood of $\mathbf{x_0}$.
- Let $X \sim U([-1,1]^d)$.

Dimension p	1	2	5	10
$P(X \in B_p(\mathbf{0_p}, 1))$	1	0.79	0.16	0.0025

- One way to overcome this problem is to work with extremely large sample sizes.

  Attention: For some problems, to have $842,000$ data in dimension 10 is really like to have 4 data in dimension 1.
- Therefore it is recommended not to go beyond 3 or 4 dimensions.
- For an explanatory variable in $\mathbb{R}^p$, it can be proved that local linear regression has $\text{AMSE}_0 = O(n^{-4/(4+p)})$.
- The higher the dimension p of explanatory variable, the lower the precision with which the regression function is estimated.
- There exist proposals alternative to local polynomial regression that overcome the curse of dimensionality: Additive models and Projection pursuit are two of them.

Additive models

- Additive models: nonparametric regression models that are less flexible than the multiple nonparametric regression model that we have seen before.
- They can be estimated with good practical results even when the number of explanatory variables is high: They are able to overcome the curse of dimensionality problem.
- Moreover the estimation results are more easily interpreted than in the case of the multiple nonparametric regression model.

- Additive model:

$$y_i = \alpha + \sum_{j=1}^{p} g_j(x_{ij}) + \varepsilon_i,$$

$$E(\varepsilon_i) = 0,\ V(\varepsilon_i) = \sigma^2,\ i = 1, \ldots, n.\ E(g_j(X_j)) = 0,\ j = 1, \ldots, p\ .$$

- Functions g_j must be estimated nonparametricaly because no parametric model is specified for them.
- The main assumption in this model is that the nonparametric univariate functions g_j are combined additively to produce the nonparametric p-dimensional regression function.
- The additive model is halfway between the multiple linear regression model (which additively combines linear transformations of the explanatory variables: $\beta_j x_{ij}$) and the multiple nonparametric regression model.

- Multiple linear regression model:

$$y_i = \alpha + \sum_{j=1}^{p} \beta_j x_{ij} + \varepsilon_i.$$

- Additive model:

$$y_i = \alpha + \sum_{j=1}^{p} g_j(x_{ij}) + \varepsilon_i.$$

- Multiple nonparametric regression model:

$$y_i = m(x_{i1}, \ldots, x_{ip}) + \varepsilon_i.$$

Estimating the additive model

- Additive model: $y_i = \alpha + \sum_{j=1}^{p} g_j(x_{ij}) + \varepsilon_i$.
- Observe that $E(y_i) = \alpha$, because $E(\varepsilon_i) = 0$ and $E(g_j(X_j)) = 0$.
- Assume for a moment that the parameter α and all functions g_j, except g_k, were known.
- In this case the unknown function g_k could be estimated by using any nonparametric univariate smoother (i.e., a local linear fit).
- It would be enough to apply the smoother to data $(x_{ik}, y_i^{(k)})$, where

$$y_i^{(k)} = y_i - \alpha - \sum_{j=1, j \neq k}^{p} g_j(x_{ij}).$$

- This reasoning leads to propose the algorithm known as backfitting to estimate the additive model.

Backfitting algorithm

- Estimate α by $\hat{\alpha} = (1/n)\sum_{i=1}^{n} y_i$.
- Take an arbitrary function $\hat{g}_k = g_k^0$ as initial estimate of function g_k, for $k = 1, \ldots, p$ (for instance, $g_k^0(x_{ik}) = \hat{\beta}_k x_{ik}$, where the coefficients $\hat{\beta}_k$ are the multiple linear regression estimated coefficients).
- REPEAT

  FOR EACH $k = 1, \ldots, p$,

  estimate g_k by a univariate smoothing of the data $(x_{ik}, y_i^{(k)})$, where

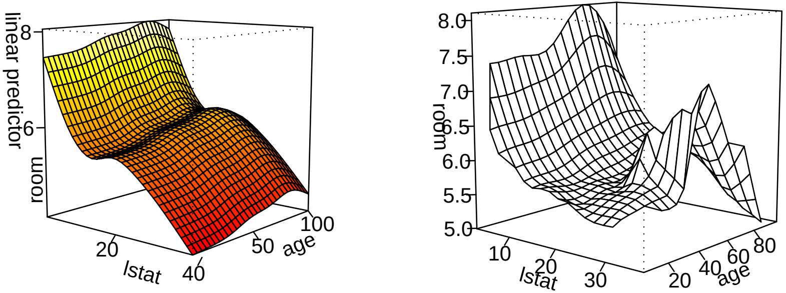
$$y_i^{(k)} = y_i - \hat{\alpha} - \sum_{j=1, j \neq k}^{p} \hat{g}_j(x_{ij}).$$

  END FOR

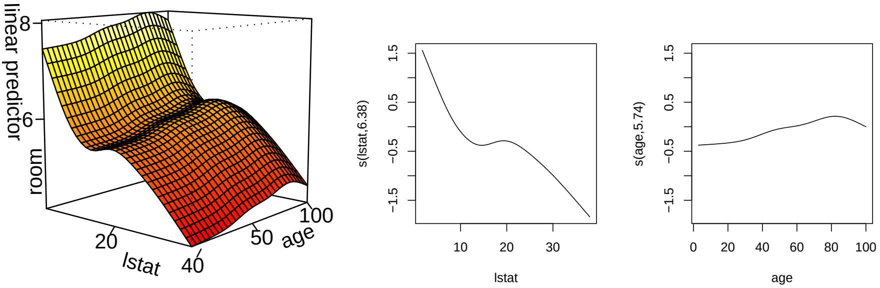
  UNTIL convergence.

Example: Boston housing data, additive model.

`ROOM` as an additive function of `LSTAT` and `AGE`.



The additive model can not pick up the local maximum (located around `LSTAT` = 35, tt AGE = 50) because it is more rigid than the nonparametric regression model.



- Axis labels show the equivalent number of parameters of both univariate estimates.
- If we cut the three-dimensional graph with cuts parallel to the plane ($\mathtt{LSTAT}$, $\mathtt{ROOM}$), the profiles that are obtained are copies of $g_{\mathtt{LSTAT}}(\cdot)$. Analogous results if the cuts are parallel to the plane ($\mathtt{AGE}$, $\mathtt{ROOM}$).
- The surface can be obtained by shifting the function $g_{\mathtt{LSTAT}}$ over the function $g_{\mathtt{AGE}}(\cdot)$ (or vice versa) and adding the mean of $\mathtt{ROOM}$.

Practice:

Additive models

Projection pursuit

- The *projection pursuit* nonparametric regression model is:

$$y_i = \alpha + \sum_{j=1}^{M} g_j(\alpha_j^T \mathbf{x_i}) + \varepsilon_i,$$

  with $E(\varepsilon_i) = 0$ and $V(\varepsilon_i) = \sigma^2$ for all $i = 1, \ldots, n$, and each α_j is a unit norm vector in $\mathbb{R}^p$.
- Moreover it is assumed that $E(g_j(\alpha_j^T \mathbf{x})) = 0$ for all $j = 1, \ldots, M$.
- Each $z_j = \alpha_j^T \mathbf{x}$ is the projection of vector $\mathbf{x}$ in the direction of vector α_j.
- The model can be written as an additive model with explanatory variables $z_1, \ldots, z_M$.
- The model look for directions α_j that maximize the explained variance of y_i.
- This is the reason for naming it *projection pursuit*.

Projection pursuit fitting algorithm

Step 1. Let $j = 1$, $\hat{\alpha} = \bar{y}_n$ and $\hat{\varepsilon}_i = y_i - \hat{\alpha}$.

Step 2. Find the direction $\hat{\alpha}_j$ minimizing

$$RSS(\alpha_j) = \sum_{i=1}^{n} (\hat{\varepsilon}_i - \hat{g}(\alpha_j^T \mathbf{x_i}))^2,$$

where $\hat{g}$ is a nonparametric estimator for the regression of $\hat{\varepsilon}_i$ as a function of $\alpha_j^T \mathbf{x_i}$. Let $\hat{g}_j$ be the function $\hat{g}$ corresponding to the optimal value $\hat{\alpha}_j$.

Step 3. Update the residuals, $\hat{\varepsilon}_i = \hat{\varepsilon}_i - \hat{g}_j(\hat{\alpha}_j^T \mathbf{x_i})$, and do $j = j + 1$.

Step 4. Return to Step 2 if the stopping rules are not fulfilled:

(a) Stop if $j = M$.

(b) Stop if $RSE(\hat{\alpha}_j)/\sum_{i=1}^{n}(y_i - \bar{y}_n)^2 < \delta$.

The values M and/or δ can be chosen by cross-validation.

Practice:

Projection pursuit regression

Generalized nonparametric multiple regression model

- The r.v. $(Y; \mathbf{X})$, with $\mathbf{X} = (X_1, \ldots, X_p)$, has distribution such that
$$(Y|\mathbf{X} = (x_1, \ldots, x_p)) \sim f(y; m(x_1, \ldots, x_p), \psi)$$
where $m(x_1, \ldots, x_p) = E(Y|\mathbf{X} = (x_1, \ldots, x_p))$ is a smooth function of $(x_1, \ldots, x_p)$, possibly subject to certain constrains (non-negativity or boundedness, for instance), and ψ represents other parameters (variance, for instance) not depending on $(x_1, \ldots, x_p)$.
- There exists an invertible link function $g(\cdot)$ such that
$$\theta(x_1, \ldots, x_p) = g(m(x_1, \ldots, x_p)), \quad m(x_1, \ldots, x_p) = g^{-1}(\theta(x_1, \ldots, x_p))$$
where $\theta(x_1, \ldots, x_p)$ is a smooth function of $(x_1, \ldots, x_p)$ free of constrains ($\theta(x_1, \ldots, x_p)$ can take any real value).
- Alternatively, $(Y|\mathbf{X} = (x_1, \ldots, x_p)) \sim f_2(y; \theta(x_1, \ldots, x_p), \psi) = f(y; g^{-1}(\theta(x_1, \ldots, x_p), \psi))$.

Generalized additive models (GAM)

- The nonparametric estimation of θ and m by maximum local likelihood also suffers the effects of the curse of dimensionality.
- A possible solution. The Generalized additive model:

$$(Y|X = (x_1, \ldots, x_p)) \sim f_2(y|\theta(x_1, \ldots, x_p), \psi), \ \theta(x_1, \ldots, x_p) = \alpha + \sum_{j=1}^{p} g_j(x_j).$$

- If the restriction that the functions g_j are linear is added, we obtain the Generalized linear model.
- Then the Generalized additive model is halfway between the Generalized nonparametric multiple regression model and the Generalized linear model.

- Generalized Linear Model:

$$(Y|X=(x_1,\ldots,x_p)) \sim f_2(y|\theta(x_1,\ldots,x_p),\psi),\ \theta(x_1,\ldots,x_p)=\alpha+\sum_{j=1}^{p}\beta_j x_j.$$

- Generalized Additive Model:

$$(Y|X=(x_1,\ldots,x_p)) \sim f_2(y|\theta(x_1,\ldots,x_p),\psi),\ \theta(x_1,\ldots,x_p)=\alpha+\sum_{j=1}^{p}g_j(x_j).$$

- Generalized nonparametric multiple regression model:

$$(Y|X=(x_1,\ldots,x_p)) \sim f_2(y|\theta(x_1,\ldots,x_p),\psi),\ \theta(x_1,\ldots,x_p) \text{ arbitrary.}$$

GAM Estimation

- The estimation of a Generalized additive model combines the backfitting algorithm (used to fit additive models) with the IRWLS algorithm (used to maximize the likelihood in GLM).
- In the IRWLS algorithm, each multiple linear regression fit by WLS is replaced by the fitting of an additive model using backfitting.
- This way the model finally fitted is a GAM instead of a GLM.

Local scoring algorithm for logistic GAM

(Source: Algorithm 9.2 in Hastie, Tibshirani, and Friedman 2001)

1. Compute starting values: $\hat{\alpha} = \log[\bar{y}/(1-\bar{y})]$, where $\bar{y}$ is the sample proportion of ones, and set $\hat{f}_j = 0$ for all j.
2. Define $\hat{\eta}_i = \hat{\alpha} + \sum_j \hat{f}_j(x_{ij})$ and $\hat{p}_i = \exp(\hat{\eta}_i)/[1+\exp(\hat{\eta}_i)]$.
   Iterate:
   (a) Construct the working target variable $z_i = \hat{\eta}_i + \frac{(y_i-\hat{p}_i)}{\hat{p}_i(1-\hat{p}_i)}$.
   (b) Construct weights $w_i = \hat{p}_i(1-\hat{p}_i)$.
   (c) Fit an additive model to the targets z_i with explanatory variables x_{ij} and weights w_i, using a weighted backfitting algorithm. This gives new estimates $\hat{\alpha}$, $\hat{f}_j$, $\forall j$.
3. Repeat step 2 until the change in the functions falls below a prespecified threshold.

Semiparametric models

- Sometimes some of the explanatory variables involved in the definition of a generalized additive model (or an additive model) affect the response variable linearly.
- If this is known in advance, the GAM model can be reformulated allowing some of the functions $g_j(x_j)$ to be linear: $g_j(x_j) = \beta_j x_j$.
- Other possible modifications of the GAM model are:
  - Nonparametrically estimating the combined effect of two (or more) explanatory variables. This includes, for example, replacing $g_j(x_j) + g_h(x_h)$ by $g_{j,h}(x_j, x_h)$.
  - Estimating the effect of a variable x_j differently at each of the classes determined by another categorical variable x_h. These effects could be estimated linearly or nonparametrically.

Semiparametric models. References

- The models obtained by incorporating these modifications to the GAM model are known as Semiparametric models.
- These models can be fitted using the function `gam` in the R package `mgcv`, developed by S. Wood (see Wood 2006).
- The book Ruppert, Wand, and Carroll (2003) is entirely dedicated to semiparametric models.
- These authors have developed in parallel the R package `SemiPar`, that allows fitting these models.
- Specifically, function `spm` has similarities with function `gam` in `mgcv`, but it incorporates additional options.

Practice:

Generalized additive models and semiparametric models

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