

```
logLik.bamlss <- function(object, ..., optimizer = FALSE, samples = FALSE)
{
  Call <- match.call()
  Call <- Call[!(names(Call) %in% c("optimizer", "samples"))]
  mn <- as.character(Call)[-1L]
  object <- list(object, ...)
  mstop <- object$mstop
  if(any(names(object) != "")) {
    i <- names(object) == ""
    object <- object[i]
    mn <- mn[i]
  }
  object <- object[mn != "mstop"]
}
```

# Advanced Bayesian Methods: Theory and Applications in R

Penalized Spline Smoothing

Nikolaus Umlauf

<https://nikum.org/abm.html>

# Linear Models

- The work horse of statistical modelling and analysis is the linear model where

$$y_i = \mathbf{x}_i^\top \boldsymbol{\beta} = \beta_0 + \beta_1 x_{i1} + \dots + \beta_k x_{ik} + \varepsilon_i, \quad \varepsilon_i \stackrel{i.i.d.}{\sim} N(0, \sigma^2).$$

- The parameters  $\beta_j$  can be related to the expected change in the response associated with differences in  $x_j$ .  
⇒ Parameters have a specific meaning and purpose.
- Statistical inference is facilitated by the distributional assumptions on the error terms.
- However, in many practical situations the linear model is not flexible enough and/or assumptions may be questionable.

# Nonlinear Effects

- Common practice if the linearity of the effect of  $x_j$  is questionable: Include low-order polynomials, e.g. replace  $x_j\beta_j$  by

$$x_j\beta_j + x_j^2\beta_{j+1} + x_j^3\beta_{j+2}.$$

- Imposes strong assumptions on the form of the effect and is not very flexible.
- Ideally, the form of an effect should be left unspecified and should be determined by the data (under mild, qualitative assumptions).
- Additive model:

$$y_i = \beta_0 + f_1(x_{i1}) + \dots + f_k(x_{ik}) + \varepsilon_i, \quad \varepsilon_i \stackrel{i.i.d.}{\sim} N(0, \sigma^2).$$

- We will use penalized splines to represent the effects  $f_j(x_{ij})$ .

# Clustered Data

- For longitudinal data  $(y_{it}, \mathbf{x}_{it})$ ,  $i = 1 \dots, n$ ,  $t = 1, \dots, T$ , a classical model of the form

$$y_{it} = \mathbf{x}_{it}^T \boldsymbol{\beta} + \varepsilon_{it}$$

may be questionable for a number of reasons:

- Unobserved heterogeneity due to individual-specific, unobserved confounders that have not been included in the model,
- Dependence between observations on one individual, or
- Individual-specific regression coefficients.

# Clustered Data

- Similarly applies to other grouping structures (families, geographical regions, school classes, ...)
- Random effects models are then often considered, e.g. random intercepts

$$y_{it} = \gamma_{0i} + \mathbf{x}_{it}^{\top} \boldsymbol{\beta} + \varepsilon_{it}$$

with  $\gamma_{i0} \stackrel{i.i.d.}{\sim} N(0, \tau^2)$ .

- More complex models can also have individual-specific random slopes or other additional structures.

# Spatial Dependence

- For spatial regression data  $(y(s), \mathbf{x}(s))$ , one may similarly question whether linear models take unobserved spatial heterogeneity and/or dependence into account.
- Include spatially correlated random effects, leading to

$$y(s) = \gamma(s) + \mathbf{x}(s)^\top \boldsymbol{\beta} + \varepsilon(s)$$

with  $\gamma(s)$  being an appropriately specified spatial stochastic process.

# Bayesian Additive Regression

- Bayesian additive regression provides a unifying framework for dealing with the challenges discussed so far.
- The model also supports other effect types, e.g., varying coefficients or interaction surfaces.
- The models can be conveniently represented in a hierarchical fashion that enables us to benefit from the flexibility of Bayesian inference.
- Tomorrow, we will discuss Bayesian distributional regression that allows us to overcome the normality assumption for the error terms.

# Example

## **Car insurance data from two insurance companies in Belgium:**

- Sample of approximately 160.000 policyholders.
- Aims: Separate risk analyses for claim size and claim frequency to predict risk premium from covariates.
- Variables of primary interest: Claim size  $\text{amount}_i$ ; or claim frequency  $\text{nclaims}_i$  of policyholders.



# Example

Variable	Description
agec	Vehicle's age.
ageph	Policyholder's age.
power	Vehicle's horsepower.
bm	Bonus-malus score.
region, NAME_4	District in Belgium.
lon, lat	Longitude/Latitude coordinates of districts.
fleet	Vehicle belongs to a fleet ("yes", "no").
sex	Gender of the policy holder ("male", "female").
coverage	Possible other guarantees subscribed, 1 = TPL only, 2 = limited material damage or theft in addition to TPL, 3 = comprehensive coverage in addition to TPL.

# Example

- Generalised linear models:

- Gaussian model for log-costs  $\log(\text{amount})$ :

$$\log(\text{amount}) \sim N(\mathbf{x}^\top \boldsymbol{\beta}, \sigma^2).$$

- Poisson model for frequencies  $\text{nclaims}_j$ :

$$\text{nclaims} \sim Po(\exp(\mathbf{x}^\top \boldsymbol{\beta})).$$

- Linear predictors formed as a linear combination of (possibly transformed) covariates:

$$\eta = \mathbf{x}^\top \boldsymbol{\beta} = \beta_0 + x_1 \beta_1 + \dots + x_p \beta_p.$$

# Example

- Subject-matter knowledge:
  - Young and old drivers have a higher claims expenditure. This hints at a quadratic instead of a linear age effect, but the precise form is unknown.  
⇒ Replace the parametric effect with a nonparametric effect  $f(\text{ageph})$ .
  - Male and female drivers have a different claims expenditure. This hints at an interaction between age and gender, but the effect should be allowed to vary with age.  
⇒ Instead of a parametric model of the form  $\beta_1 \text{ageph} + \beta_2 \text{sex} + \beta_3 \text{ageph} \cdot \text{sex}$  consider a model of the form  $f_1(\text{ageph}) + f_2(\text{ageph}) \cdot \text{sex}$ .

# Example

- Drivers in rural areas cause less accidents with a higher average claim amount while drivers in urban areas cause more but smaller claims. The effect may change smoothly between rural and urban areas such that modeling based on a rural vs. urban dummy is too simplistic.  
⇒ Include a spatial function  $f_{spat}(\text{NAME}_4)$  based on the region  $\text{NAME}_4$  a driver is living in.

# Example

- Model specifications:
  - Gaussian model for log-costs  $\log(\text{amount})$ :

$$\log(\text{amount}) \sim N(\eta, \sigma^2)$$

with

$$\eta = f_1(\text{agec}) + f_2(\text{ageph}) + f_3(\text{bm}) + f_4(\text{power}) + f_{\text{spat}}(\text{NAME\_4}) + \mathbf{x}^\top \boldsymbol{\beta}.$$

- Poisson model for frequencies  $\text{nclaims}_j$ :

$$\text{nclaims} \sim Po(\exp(\eta))$$

with

$$\eta = f_1(\text{agec}) + f_2(\text{ageph}) \cdot \text{sex} + f_3(\text{bm}) + f_4(\text{power}) + f_{\text{spat}}(\text{NAME\_4}) + \mathbf{x}^\top \boldsymbol{\beta}.$$

# Scatterplot Smoothing

- Start from scatterplot smoothing

$$y_i = f(z_i) + \varepsilon_i, \quad \varepsilon_i \stackrel{\text{i.i.d.}}{\sim} \text{N}(0, \sigma^2)$$

where  $f(z)$  should be inferred based on observations  $(z_i, y_i)$ ,  $i = 1, \dots, n$ , for a continuous covariate  $z$  and response  $y$ .

- Common approach: Approximate  $f(z)$  by a low-order polynomial

$$f(z_i) = \gamma_0 + \gamma_1 z_i + \dots + \gamma_l z_i^l$$

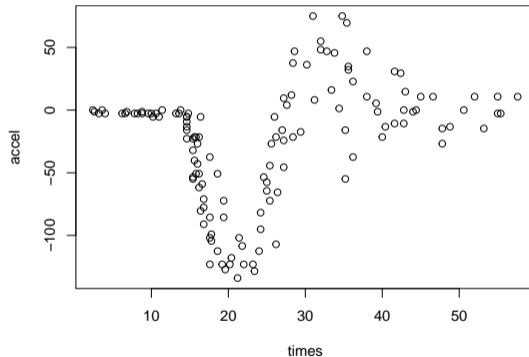
since any smooth function  $f(\cdot)$  can be approximated arbitrarily accurately if the degree  $l$  is chosen large enough.

# Scatterplot Smoothing

- In statistics, the problem of estimating the coefficients  $\gamma_0, \dots, \gamma_l$  limits the applicability of high polynomial degrees:

# Scatterplot Smoothing

```
R> data("mcycle", package = "MASS")  
R> par(mar = c(4, 4, 0, 0))  
R> plot(mcycle)
```





# Polynom Splines

- If a linear fit is too simple we could use a polynomial model

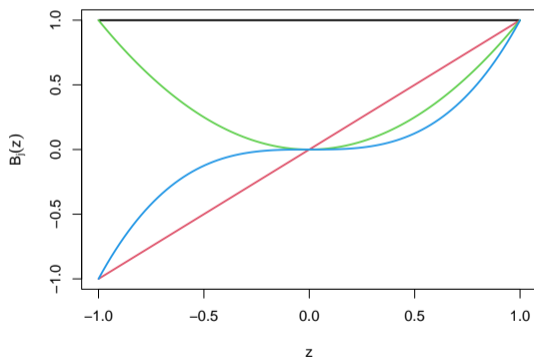
$$\text{accel}_i = \gamma_0 + \gamma_1 \text{times}_i + \dots + \gamma_l \text{times}_i^l.$$

- The parameters can be estimated by ordinary least squares.
- Note that we write  $\gamma$  instead of  $\beta$  to better distinguish between simple linear and nonlinear effects here.
- The design matrix has the following form

$$\mathbf{Z} = \begin{pmatrix} 1 & \text{times}_1 & \dots & \text{times}_1^l \\ \vdots & \vdots & \vdots & \vdots \\ 1 & \text{times}_n & \dots & \text{times}_n^l \end{pmatrix}$$

# Polynom Splines

- The columns of  $Z$  are also called basis functions  $B_j(z)$ ,  $j = 0, \dots, l$ . In this case a polynomial basis.
- With sorted  $z$  they have a nice visual representation.



# Polynom Splines

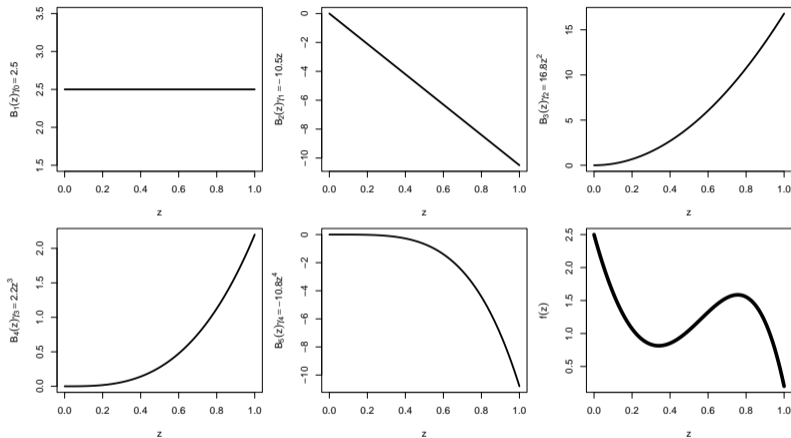
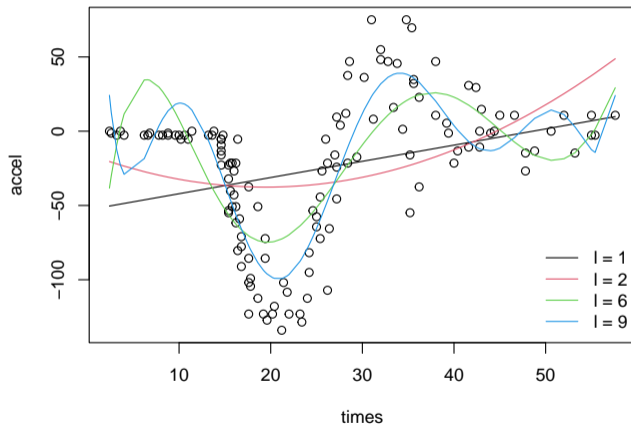


Illustration of how  $f(z)$  is represented in terms of  $B_j(z)\gamma_j$ .

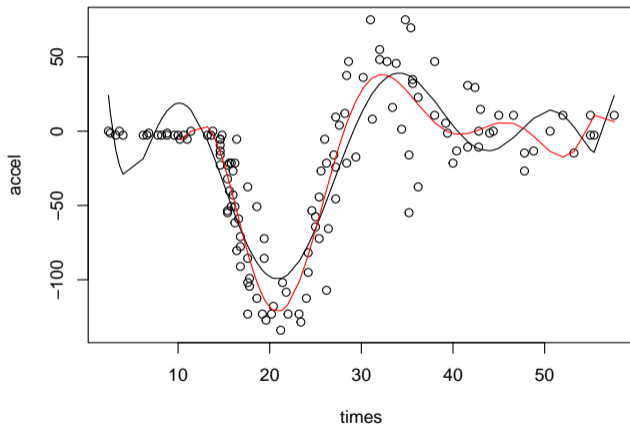
# Polynom Splines

Effect of increasing the degree  $l$  of the polynomial.



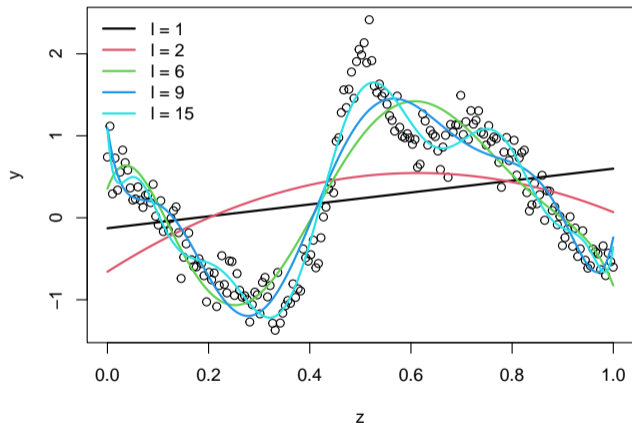
# Polynom Splines

Polynomial boundary effects.



# Polynom Splines

Effect of increasing the degree  $l$  of the polynomial.



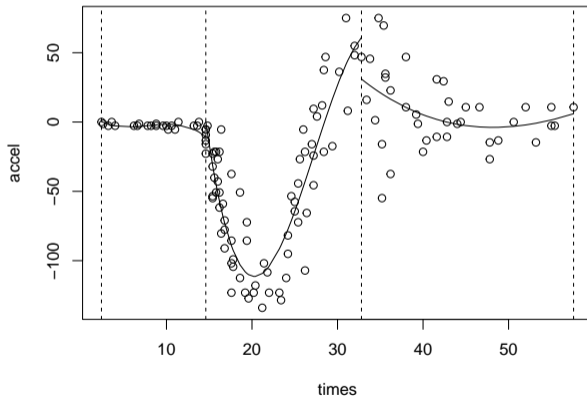
# Polynom Splines

## Problems:

- High degree needed for decent curve fit.
- Higher degree polynomials are numerically unstable.
- Basis functions are global.
- Unexpected wiggles.
- Round-off problems with  $\hat{\gamma} = (\mathbf{Z}^\top \mathbf{Z})^{-1} \mathbf{Z}^\top \mathbf{y}$ .
- Partial remedy: center and normalize  $z$ .
- Better use orthogonal polynomials instead, see also function `poly()`.

# Polynom Splines

Divide the range of  $z$  in equidistant intervals with boundaries  $\kappa$  (knots) and fit polynomial models within each section.





# Polynom Splines

- The fitted functions don't form a nice overall smooth function, see the jumps at the boundaries.
- We need additional requirements to construct a smooth functional form.

A function  $f$  is called polynomial spline of degree  $l \geq 0$  with knots  $\min(z) = \kappa_1 < \dots < \kappa_m = \max(z)$  (the interval boundaries), if it satisfies

- ①  $f(z)$  is  $(l - 1)$  times continuously differentiable,
- ②  $f(z)$  is a polynomial of degree  $l$  in each interval  $[\kappa_j, \kappa_{j+1})$ .

Every spline may be represented by a linear combination of basis functions, i.e.

$$f(z_i) = \gamma_1 \cdot B_1(z_i) + \gamma_2 \cdot B_2(z_i) + \dots + \gamma_{l+m-1} \cdot B_{l+m-1}(z_i).$$

# Polynom Splines

## Polynom splines with truncated powers

- Regression model

$$y_i = \gamma_1 + \gamma_2 z_i + \dots + \gamma_{l+1} z_i^l + \sum_{j=2}^{m-1} \gamma_{l+j} (z_i - \kappa_j)_+^l + \varepsilon_i.$$

where

$$(z_i - \kappa_j)_+^l = \begin{cases} (z_i - \kappa_j)^l & z_i \geq \kappa_j \\ 0 & \text{else.} \end{cases}$$

- Corresponding basis functions

$$B_1(z_i) = 1, \quad B_2(z_i) = z_i, \quad \dots, \quad B_{l+1}(z_i) = z_i^l, \\ B_{l+2}(z_i) = (z_i - \kappa_2)_+^l, \quad \dots, \quad B_k(z_i) = (z_i - \kappa_{m-1})_+^l.$$

# Polynom Splines

- Model using basis function representation

$$y_i = f(z_i) + \varepsilon_i = \sum_{j=1}^k \gamma_j B_j(z_i) + \varepsilon_i.$$

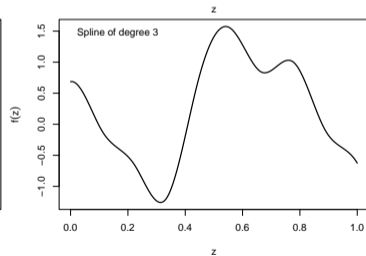
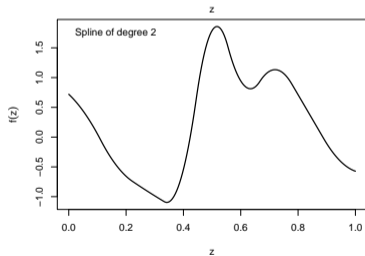
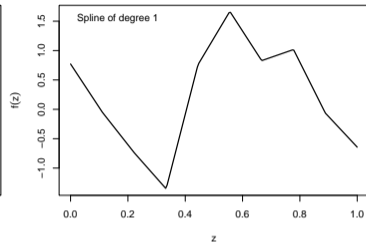
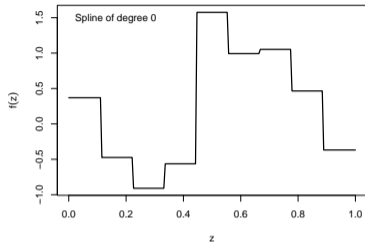
- The corresponding design matrix is

$$\mathbf{Z} = \begin{pmatrix} B_1(z_1) & \dots & B_k(z_1) \\ \vdots & & \vdots \\ B_1(z_n) & \dots & B_k(z_n) \end{pmatrix} = \begin{pmatrix} 1 & z_1 & \dots & z_1' & (z_1 - \kappa_2)'_+ & \dots & (z_1 - \kappa_{m-1})'_+ \\ \vdots & & & & & & \vdots \\ 1 & z_n & \dots & z_n' & (z_n - \kappa_2)'_+ & \dots & (z_n - \kappa_{m-1})'_+ \end{pmatrix},$$

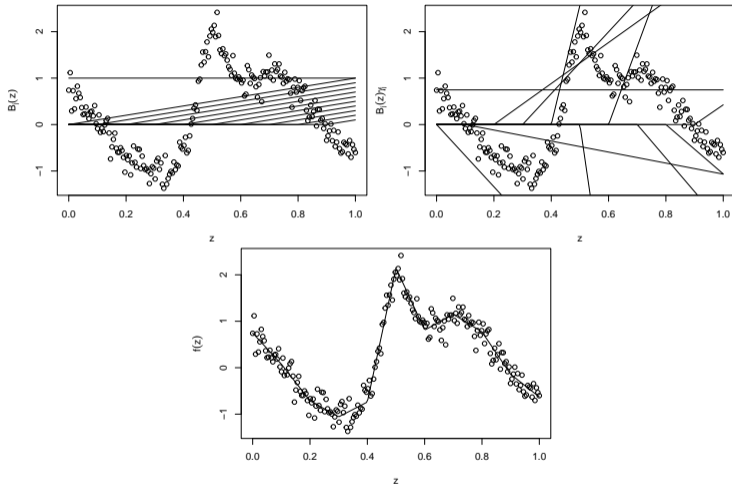
- In matrix notation

$$\mathbf{y} = \mathbf{Z}\boldsymbol{\gamma} + \boldsymbol{\varepsilon} \text{ and } \hat{\boldsymbol{\gamma}} = (\mathbf{Z}^\top \mathbf{Z})^{-1} \mathbf{Z}^\top \mathbf{y}.$$

# Polynom Splines



# Polynom Splines



# Penalized Regression

- Although most of the automatic knot selection procedures have exhibited good performance, they are usually quite complicated and computational intensive.
- We therefore seek a simpler method for flexible spline-based regression.
- As mentioned before, the roughness of a fit is due to there being too many knots in the model.
- Another way to overcome this problem is to retain all of the knots but to constrain their influence.
- The hope is that this will result in a less variable fit.

# Penalized Regression

## Penalized Regression with TP-Splines:

- Consider the truncated polynomial model

$$f(z_i) = \gamma_1 + \gamma_2 z_i + \dots + \gamma_{l+1} z_i^l + \sum_{j=2}^{m-1} \gamma_{l+j} (z_i - \kappa_j)_+^l.$$

- The wiggleness of the fit is mainly the result of too large variability of the coefficients of the truncated bases.
- Constraints on the  $\gamma_{l+j}$  that might rectify this situation are
  - ①  $\max |\gamma_{l+j}| < C,$
  - ②  $\sum |\gamma_{l+j}| < C,$  and
  - ③  $\sum \gamma_{l+j}^2 < C.$
- Each of these will lead to a smoother fit, however, the third constraint is much easier to implement.

# Penalized Regression

- Define the  $((m - 2) + l) \times ((m - 2) + l)$  matrix

$$\mathbf{K} = \begin{pmatrix} \mathbf{0}_{l \times l} & \mathbf{0}_{l \times (m-2)} \\ \mathbf{0}_{(m-2) \times l} & \mathbf{I}_{(m-2) \times (m-2)} \end{pmatrix},$$

then our minimization problem can be written as

$$\min \|\mathbf{y} - \mathbf{Z}\boldsymbol{\gamma}\|^2 \text{ subject to } \boldsymbol{\gamma}^\top \mathbf{K} \boldsymbol{\gamma} < C.$$

- Using a Lagrange multiplier argument, it can be shown that this is equivalent to choosing  $\boldsymbol{\gamma}$  to minimize

$$\|\mathbf{y} - \mathbf{Z}\boldsymbol{\gamma}\|^2 + \lambda \boldsymbol{\gamma}^\top \mathbf{K} \boldsymbol{\gamma}$$

for some  $\lambda \geq 0$ .



# Penalized Regression

- The solution is then given by

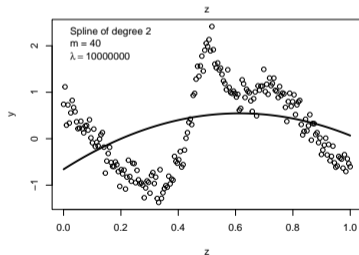
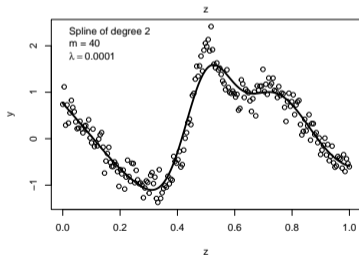
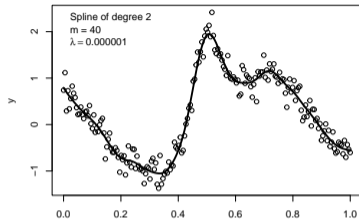
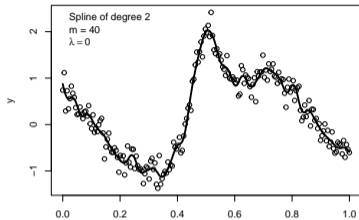
$$\hat{\boldsymbol{\gamma}} = \left( \mathbf{Z}^T \mathbf{Z} + \lambda \mathbf{K} \right)^{-1} \mathbf{Z}^T \mathbf{y}.$$

- The fitted values for a penalized spline regression are

$$\hat{\mathbf{y}} = \mathbf{Z} \left( \mathbf{Z}^T \mathbf{Z} + \lambda \mathbf{K} \right)^{-1} \mathbf{Z}^T \mathbf{y} = \mathbf{S}_\lambda \mathbf{y},$$

where  $\mathbf{S}_\lambda$  is called smoother matrix.

# Penalized Regression



# P-Splines

- Truncated power bases can sometimes lead to numerical instability when there is a large number of knots and the smoothing parameter is small.
- Therefore, in practical use it is advisable to work with equivalent bases with more stable numerical properties.
- The most common choice is the B-spline basis.
- B-spline basis can represent cubic splines (and also higher or lower orders).
- The advantage of B-splines is that they are strictly local – each basis function is only non-zero over  $l + 1$  adjacent knots.

# P-Splines

- To define a B-spline with  $k$  basis functions we need to set up  $m + l + 1$  knots

$$\kappa_1 < \kappa_2 < \dots < \kappa_{m+l+1},$$

where the interval over which the spline is to be evaluated is  $[\kappa_{l+1}, \kappa_k]$ , i.e., the first and the last  $l$  knot locations are essentially arbitrary.

- Every basis function overlaps with  $2l$  neighboring basis functions and is positive over  $l + 2$  neighboring knots.
- The B-spline is  $l - 1$  times continuously differentiable.
- A  $l$ th order B-spline is then represented by

$$f(z_i) = \sum_{j=1}^k B_j^l(z_i) \gamma_j.$$

# P-Splines

- The B-spline basis functions are most conveniently defined recursively as follows:

$$B_j^l(z_i) = \frac{z_i - \kappa_j}{\kappa_{j+l} - \kappa_j} B_j^{l-1}(z_i) + \frac{\kappa_{j+l+1} - z_i}{\kappa_{j+l+1} - \kappa_{j+1}} B_{j+1}^{l-1}(z_i),$$

- where

$$B_j^0(z_i) = \begin{cases} 1 & \kappa_j \leq z_i < \kappa_{j+1}, \\ 0 & \text{else.} \end{cases}$$

- A common choice is a cubic spline basis with  $l = 3$ .

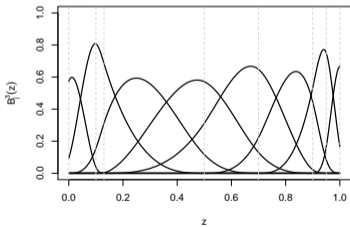
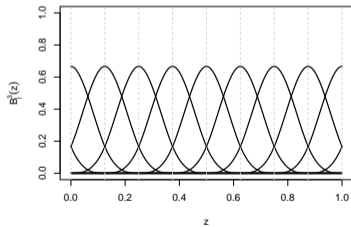
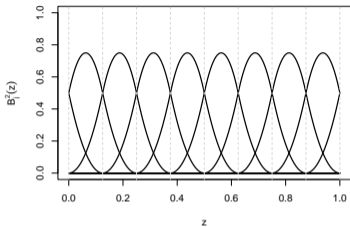
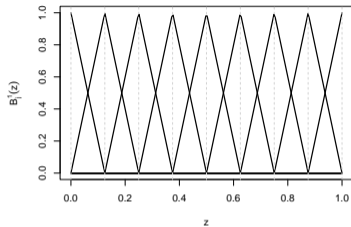
# P-Splines

```
R> ## Evaluate a B-spline design matrix
R> ## first, define the B-spline basis function
R> ## recursively.
R> bsbasis <- function(z, knots, j, degree) {
+   if(degree == 0)
+     B <- 1 * (knots[j] <= z & z < knots[j + 1])
+   if(degree > 0) {
+     b1 <- (z - knots[j]) / (knots[j + degree] - knots[j])
+     b2 <- (knots[j + degree + 1] - z) /
+       (knots[j + degree + 1] - knots[j + 1])
+     B <- b1 * bsbasis(z, knots, j, degree - 1) +
+       b2 * bsbasis(z, knots, j + 1, degree - 1)
+   }
+   B[is.na(B)] <- 0
+   return(B)
+ }
```

# P-Splines

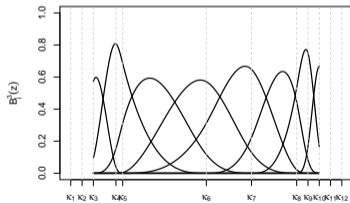
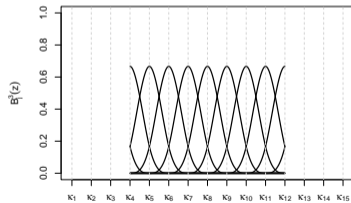
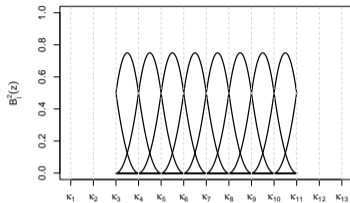
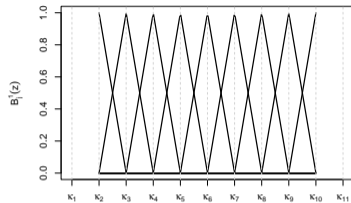
```
R> ## Now, compute the design matrix for all knots.
R> bsDesign <- function(z, degree = 3, knots = NULL) {
+   ## Compute knots.
+   if(is.null(knots))
+     knots <- 40
+   if(length(knots) < 2) {
+     step <- (max(z) - min(z)) / (knots - 1)
+     knots <- seq(min(z) - degree * step,
+                 max(z) + degree * step, by = step)
+   }
+
+   ## Evaluate each basis function
+   ## and return the full design matrix B.
+   B <- NULL
+   for(j in 1:(length(knots) - degree - 1))
+     B <- cbind(B, bsbasis(z, knots, j, degree))
+   return(B)
+ }
```

# P-Splines

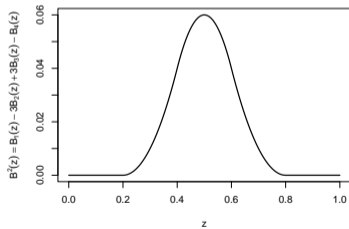
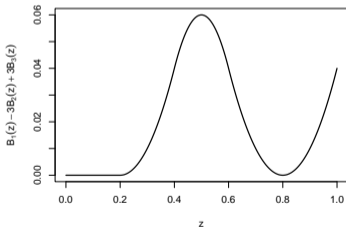
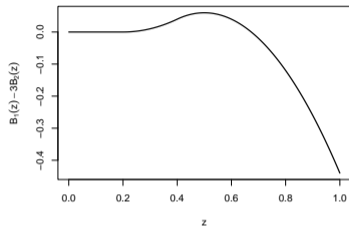
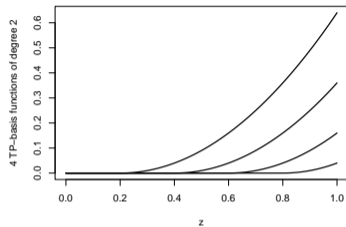




# P-Splines



# P-Splines



# P-Splines

- With B-spline basis functions a penalty on the regression coefficients is not obvious, since we do not divide in a parametric and non-parametric part.
- Since we want an overall smooth function we could use the following penalty

$$\lambda \int (f''(z))^2 dz.$$

- For B-splines we can construct simpler equivalent penalty terms

$$\|\mathbf{y} - \mathbf{Z}\boldsymbol{\gamma}\|^2 + \lambda \boldsymbol{\gamma}^\top \mathbf{K} \boldsymbol{\gamma}$$

with

$$\lambda \boldsymbol{\gamma}^\top \mathbf{K} \boldsymbol{\gamma} = \sum_{j=k+1}^k (\Delta^d \gamma_j)^2.$$

# P-Splines

- $\Delta^d$  is the  $d$ th order difference which is defined recursively

$$\Delta^1 \gamma_j = \gamma_j - \gamma_{j-1}$$

$$\Delta^2 \gamma_j = \Delta^1 \Delta^1 \gamma_j = \Delta^1 \gamma_j - \Delta^1 \gamma_{j-1} = \gamma_j - 2\gamma_{j-1} + \gamma_{j-2}$$

$$\vdots$$

$$\Delta^d \gamma_j = \Delta^{d-1} \gamma_j - \Delta^{d-1} \gamma_{j-1}.$$

- The first order difference matrix is then given by

$$\mathbf{D}_1 = \begin{pmatrix} -1 & 1 & & & \\ & -1 & 1 & & \\ & & \ddots & \ddots & \\ & & & -1 & 1 \end{pmatrix} \quad \text{with } \mathbf{D}_1 \boldsymbol{\gamma} = \begin{pmatrix} \gamma_2 - \gamma_1 \\ \vdots \\ \gamma_k - \gamma_{k-1} \end{pmatrix}.$$

# P-Splines

- The difference matrices can be computed recursively with

$$\mathbf{D}_d = \mathbf{D}_1 \mathbf{D}_{d-1}.$$

- Now, the resulting penalty matrix  $\mathbf{K}$  is

$$\mathbf{K} = \mathbf{D}_k^T \mathbf{D}_k.$$

```
R> ## Penalty matrix based on difference matrices.  
R> penalty <- function(order = 2, k = 10) {  
+   D <- diag(k)  
+   for(i in 1:order)  
+     D <- diff(D)  
+   K <- crossprod(D, D)  
+   return(K)  
+ }
```

# P-Splines

```
R> penalty(order = 1)
```

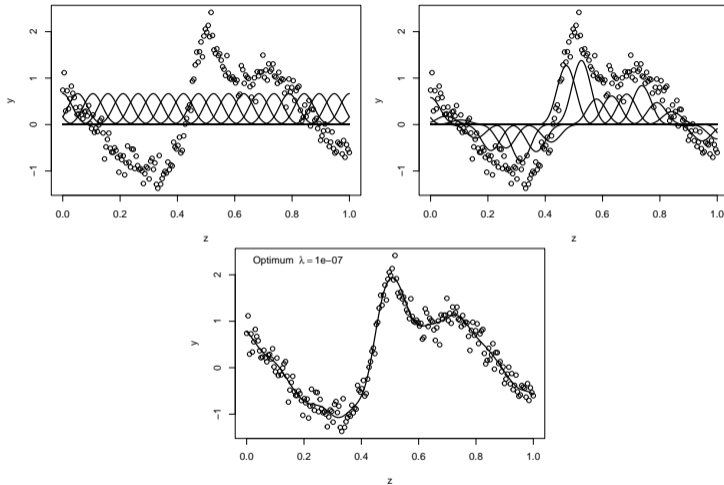
	[,1]	[,2]	[,3]	[,4]	[,5]	[,6]	[,7]	[,8]	[,9]	[,10]
[1,]	1	-1	0	0	0	0	0	0	0	0
[2,]	-1	2	-1	0	0	0	0	0	0	0
[3,]	0	-1	2	-1	0	0	0	0	0	0
[4,]	0	0	-1	2	-1	0	0	0	0	0
[5,]	0	0	0	-1	2	-1	0	0	0	0
[6,]	0	0	0	0	-1	2	-1	0	0	0
[7,]	0	0	0	0	0	-1	2	-1	0	0
[8,]	0	0	0	0	0	0	-1	2	-1	0
[9,]	0	0	0	0	0	0	0	-1	2	-1
[10,]	0	0	0	0	0	0	0	0	-1	1

# P-Splines

```
R> penalty(order = 2)
```

	[,1]	[,2]	[,3]	[,4]	[,5]	[,6]	[,7]	[,8]	[,9]	[,10]
[1,]	1	-2	1	0	0	0	0	0	0	0
[2,]	-2	5	-4	1	0	0	0	0	0	0
[3,]	1	-4	6	-4	1	0	0	0	0	0
[4,]	0	1	-4	6	-4	1	0	0	0	0
[5,]	0	0	1	-4	6	-4	1	0	0	0
[6,]	0	0	0	1	-4	6	-4	1	0	0
[7,]	0	0	0	0	1	-4	6	-4	1	0
[8,]	0	0	0	0	0	1	-4	6	-4	1
[9,]	0	0	0	0	0	0	1	-4	5	-2
[10,]	0	0	0	0	0	0	0	1	-2	1

# P-Splines





# Bayesian P-splines

Penalized splines can also be derived in a Bayesian framework

In particular, this allows us to employ Bayesian approaches for the estimation of P-splines including the smoothing parameter.

Lets start with the observation model

$$y_i = \sum_{j=1}^d \gamma_j B_j(z_i) + \varepsilon_i \quad \varepsilon_i \sim N(0, \sigma^2),$$

with B-spline basis functions  $B_j$ .

Instead of imposing a penalty, we will now develop an appropriate prior assumption for  $\gamma$  that enforces a smooth function estimation.

# Bayesian P-splines

## Priors of regression coefficients

- The stochastic analogue for the difference penalty are *random walks* of order  $k$  (RW $k$ ).
- A random walk of first order (RW1) is defined by

$$\gamma_j = \gamma_{j-1} + u_j, \quad u_j \sim N(0, \tau^2), \quad j = 2, \dots, d,$$

or equivalently

$$\gamma_j - \gamma_{j-1} = u_j, \quad u_j \sim N(0, \tau^2), \quad j = 2, \dots, d,$$

so that a connection to the first order difference penalty is recognizable.

- We have to make further assumptions for the prior of the starting value  $\gamma_1$  and a noninformative prior distribution,  $p(\gamma_1) \propto \text{const}$  will be our standard option.

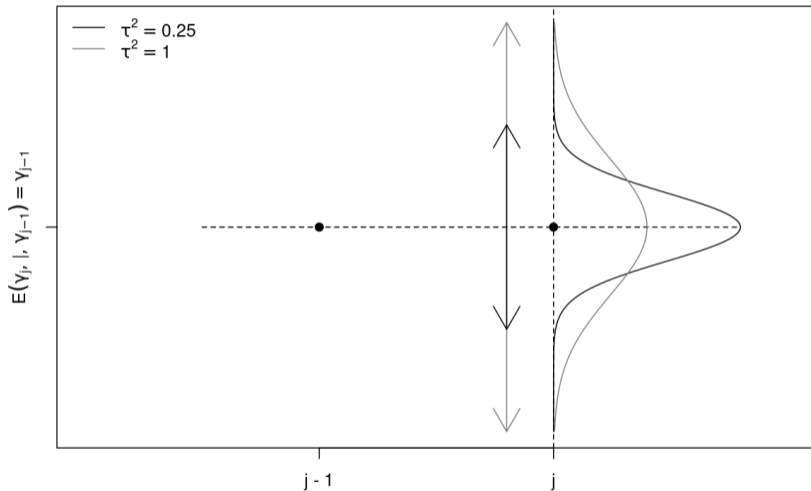
# Bayesian P-splines

- When considering the conditional distributions defined by a RW1, we have

$$\gamma_j | \gamma_{j-1}, \dots, \gamma_1 \sim N(\gamma_{j-1}, \tau^2).$$

- The RW1 has a special dependence structure such that the conditional distribution of  $\gamma_j$  given all previous values is only dependent on the value lagged by one, i.e.  $\gamma_{j-1}$ .
- Therefore, the RW1 has the (first order) *Markov property*.
- According to this formulation, the conditional expectation of  $\gamma_j$  is simply the lagged value  $\gamma_{j-1}$  such that we obtain a constant trend for the expected value.

# Bayesian P-splines



# Bayesian P-splines

- The larger the variance, the larger the possible deviation from the conditional expectation.
- A constant value of all B-spline coefficients leads to a constant estimate for the function  $f(z)$ . This corresponds to the case that the variance of the RW1 is (almost) zero, since only very little deviation between  $\gamma_j$  and  $\gamma_{j-1}$  is allowed in this situation resulting in a (near) constant trend for the sequence  $\gamma_1, \dots, \gamma_d$ .
- In contrast, when having a large variance  $\tau^2$ , neighboring coefficients are able to deviate from each other, which in turn leads to a rough estimated function.
- It follows that we can interpret the variance parameter  $\tau^2$  as related to an inverse smoothing parameter.

# Bayesian P-splines

- The joint multivariate prior distribution for  $\gamma$  is then given by

$$\begin{aligned} p(\gamma|\tau^2) &= \prod_{j=1}^d p(\gamma_j|\gamma_{j-1}, \dots, \gamma_1) = p(\gamma_1) \prod_{j=2}^d p(\gamma_j|\gamma_{j-1}) \\ &\propto \prod_{j=2}^d \frac{1}{\sqrt{2\pi\tau^2}} \exp\left(-\frac{1}{2\tau^2}(\gamma_j - \gamma_{j-1})^2\right) \\ &= \frac{1}{(2\pi\tau^2)^{(d-1)/2}} \exp\left(-\frac{1}{2\tau^2} \sum_{j=2}^d (\gamma_j - \gamma_{j-1})^2\right) \\ &= \frac{1}{(2\pi\tau^2)^{(d-1)/2}} \exp\left(-\frac{1}{2\tau^2} \gamma^\top \mathbf{K}_1 \gamma\right). \end{aligned}$$