# Module 5: Generalized Additive Models

BIOS 526

**Reading**

- From Wood, S. *Generalized Additive Models: An Introduction with R, 2nd Edition*: Chapter 4, 5.1.2, 5.3.1, 5.4, 5.5.1, 6.1.2, 6.10, 6.12.
- A nice resource for fitting GAMs: `https://wiki.qcbs.ca/r_workshop8`.

**Concepts**

- Generalized additive models (logistic).
- Additive models with multiple covariates
- Using $gam()$ in package $mgcv()$ to fit semiparametric models with parametric (slopes) and nonparametric terms (functions)
- Bivariate splines.
- Interpreting non-linear effects.

# Generalized Additive Models

# Binary Outcome Example

Recall the example from Module 4:

Dataset: a cohort of live births from Georgia born in the year 2001 (N = 77,340).

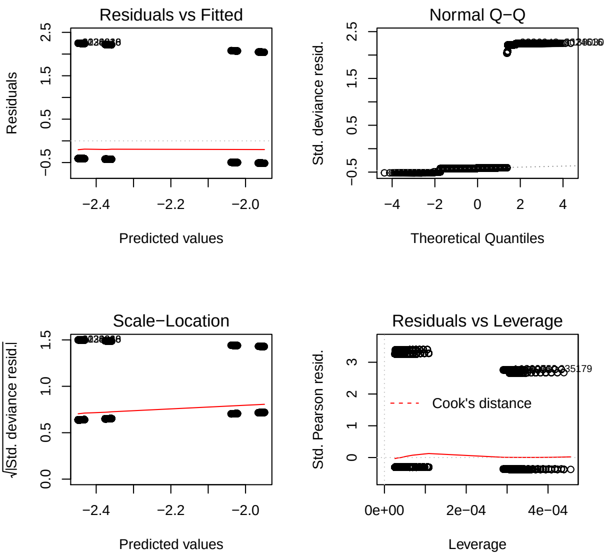
Variables:

- $ptb$: indicator for whether the baby from pregnancy $i$ was born preterm ($<$ 37 weeks).
- $age$: the mother's age at delivery.
- $male$: indicator of the baby's sex (1 = male; 0=female).
- $tobacco$: indicator for mother's tobacco use during pregnancy (1 = yes; 0 = no)

# Previous analysis

```
### Fit logistic regression model
> fit = glm(ptb~age + male+tobacco, data = dat, family = binomial(link='logit'))
> summary(fit)

Call:
glm(formula = ptb ~ age + male + tobacco, family = binomial(link = "logit"),
    data = dat)

Deviance Residuals:
       Min          1Q      Median          3Q         Max
-0.5159563  -0.4235975  -0.4102807  -0.4087970   2.2499946

Coefficients:
                Estimate   Std. Error   z value   Pr(>|z|)
(Intercept) -2.421266448  0.063135527 -38.35030 < 2.22e-16 ***
age         -0.000629473  0.002159576  -0.29148  0.7706843
maleM        0.072365862  0.025867177   2.79759  0.0051485 **
tobacco      0.409649486  0.053462733   7.66234 1.8258e-14 ***
---
Signif. codes:  0 ?***? 0.001 ?**? 0.01 ?*? 0.05 ?.? 0.1 ? ? 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 44907.564  on 77339  degrees of freedom
Residual deviance: 44845.557  on 77336  degrees of freedom
AIC: 44853.557
```

The plot diagnostics are not very helpful with binary responses:



# Generalized Additive Model

Note: when we have linear terms and smooths, sometimes called semiparametric regression

To account for non-linear age effect

$$ptd_i \overset{IND}{\sim} \text{Bernoulli}(p_i)$$

$$\text{logit}\, p_i = \beta_0 + \beta_1 \text{male}_i + \beta_2 \text{tobacco}_i + s(\text{age}_i)$$

$\log\left(\frac{p_i}{1-p_i}\right)$

where $s(age_i)$ is a smooth function of age. The above model is known as a generalized additive model.

GAMs: Generalized Additive Models.

Everything we learned about additive models is directly applicable in this setting!

# GAM with logit link

Using the mgcv::gam function:

```
> fit.gam = gam(ptb~s(age)+male+tobacco,family=binomial,data=dat)
> summary(fit.gam)

Family: binomial
Link function: logit

Formula:
ptb ~ s(age) + male + tobacco
....

Parametric coefficients:
            Estimate Std. Error  z value Pr(>|z|)
(Intercept) -2.44226    0.01913 -127.647  < 2e-16 ***
maleM        0.07274    0.02588    2.811  0.00494 **
tobacco      0.39016    0.05356    7.284 3.24e-13 ***
---
Signif. codes:  0 ?***? 0.001 ?**? 0.01 ?*? 0.05 ?.? 0.1 ? ? 1

Approximate significance of smooth terms:
         edf Ref.df Chi.sq  p-value
s(age) 3.314  4.146  70.17 3.85e-14 ***
---
Signif. codes:  0 ?***? 0.001 ?**? 0.01 ?*? 0.05 ?.? 0.1 ? ? 1

R-sq.(adj) =  0.00177   Deviance explained = 0.304%
UBRE = -0.42095  Scale est. = 1         n = 77340
```

note: actually fitting $\text{logit}[E(ptb_i)] \sim s(age_i) + male_i + tobacco_i$

$\neq 1$, indicates we have non-linear effect of age on the log odds of preterm birth

# GAM diagnostics

```
> gam.check(fit.gam)

Method: UBRE   Optimizer: outer newton
full convergence after 3 iterations.
Gradient range [9.816712095e-07,9.816712095e-07]
(score -0.4209494806 & scale 1).
Hessian positive definite, eigenvalue range [1.285936713e-05,1.285936713e-05].
Model rank =  12 / 12

Basis dimension (k) checking results. Low p-value (k-index<1) may
indicate that k is too low, especially if edf is close to k'.

          k'  edf k-index p-value
s(age) 9.00 3.31    0.94    0.66
```

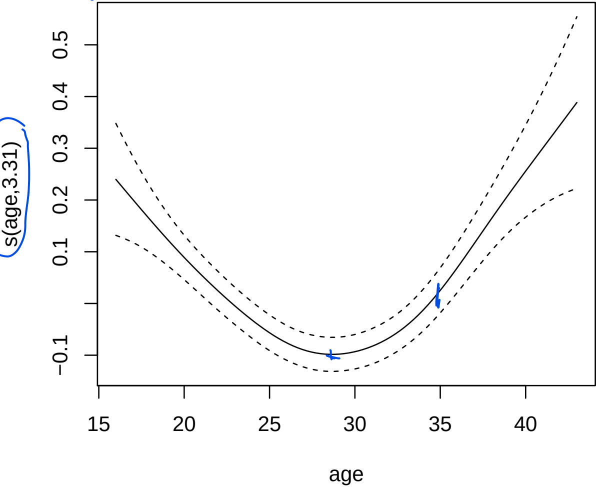
unbiased risk estimation replaces GCV when using a glm likelihood

$3.31 << 9$, suggests $k=10$ is sufficient

# Generalized Additive Model

Biologically: log odds of preterm birth is higher at very young ages, lowest around 29 years, and then increased again

effect of age on logs odds scale



# Bayesian credible intervals

We are assuming the underlying function is smooth. We can formalize this as a prior in a Bayesian model. We won't get into details, ~~but may return to this topic in M7~~.

In Bayesian statistics, the parameters $\boldsymbol{\beta}$ are random variables. A ridge penalty corresponds to an improper Gaussian prior:

A RIDGE PENALTY ≃ GAUSSIAN PRIOR

$$f_{\boldsymbol{\beta}} \propto \exp(-\boldsymbol{\beta}'\mathbf{B}\boldsymbol{\beta}/2).$$

For Gaussian data, this results in a posterior distribution

$$[\boldsymbol{\beta}|\mathbf{y}, \lambda] \sim N\left\{\hat{\boldsymbol{\beta}}, \sigma^2(\mathbf{X}'\mathbf{X} + \lambda\mathbf{B})^{-1}\right\}$$

in mgcv, estimated using GCV or REML-trick

For a general likelihood, we use the Fisher Information matrix (Hessian of the negative log likelihood at $\hat{\boldsymbol{\beta}}$)

$$[\boldsymbol{\beta}|\mathbf{y}, \lambda] \sim N\left\{\hat{\boldsymbol{\beta}}, \left(\hat{\mathcal{I}} + \lambda\mathbf{B}\right)^{-1}\right\}$$

Multiply by $\phi$ for quasi-Poisson.
In particular, the "Bayesian credible intervals" plotted in mgcv::gam have Frequentist coverage probabilities. See Section 6.10 in Wood.

# Multiple Smoothers

# Multiple Smooth Terms

Let's consider an additive model for two continuous variables, $x_i$ and $z_i$:

$$y_i = \beta_0 + g_1(x_i) + g_2(z_i) + \varepsilon_i, \quad \varepsilon_i \overset{iid}{\sim} N(0, \sigma^2)$$

where $g_1(\cdot)$ and $g_2(\cdot)$ denote smooth relationships between the response $y_i$ and predictors $x_i$ and $z_i$.

Again, extends to generalized linear models (binomial, Poisson, etc).

We again express non-linear functions using basis functions:

$$g_1(x_i) = \sum_{m=1}^{M_1} \beta_{m1} b_{m1}(x_i), \quad g_2(z_i) = \sum_{m=1}^{M_2} \beta_{m2} b_{m2}(z_i)$$

Induce smoothing by penalizing regression coefficients.

Note we also use smoothers to control for **confounders** flexibly.

# Associations between Mortality and Fine Particulate Matter

Fine particulate matter ($PM_{2.5}$):

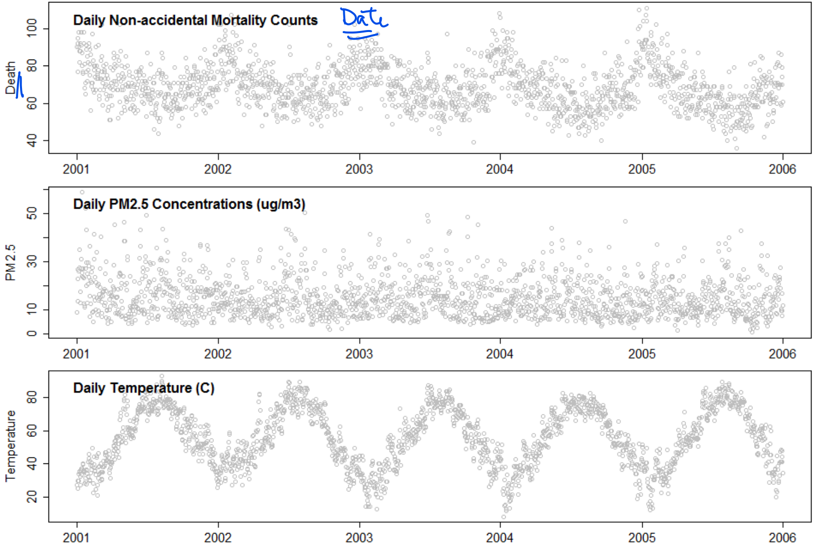
- represents a mixture of solid and liquid particles in the air that are less than 2.5 $\mu m$ in diameter;
- mainly arises from combustion sources (power generation, vehicle, and industrial operations).

Scientific Question: what is the association between daily mortality counts and daily concentration of outdoor $PM_{2.5}$ air pollution?

Data Sources:

- Daily counts of non-accidental deaths (age $\geq 65$) in the 5-county New York City area (2001-2005) obtained from the National Center for Health Statistics (CDC).
- Daily $PM_{2.5}$ concentrations from Environmental Protection Agency
- Daily meteorology conditions from the National Climatic Data Center (NOAA).

# Associations between Mortality and Fine Particulate Matter



# Time-Series Health Model

- We are interested in the association between daily variation in mortality counts and daily variation in exposure. to PM2.5
- In a time-series design we view population as the unit of analysis. I.e. outcome = total mortality counts arising from the population.
- Confounders that vary smoothly in time can be easily controlled for by including smooths.

# Time-Series Health Model

Let $y_t$ denote the death count on day $t$, and $x_t$ be the corresponding $PM_{2.5}$ level.

There is typically a *temporal delay* between exposure and outcome.

Let's examine the association between daily mortality and previous-day exposure.

time index, look at PM2.5 in previous day on mortality

log transform to meet the NORMALITY

assume independence across time in residuals

$$\log y_t = \beta_0 + g_1(x_{t-1}) + \text{confounders} + \epsilon_t \ , \quad \epsilon_t \overset{iid}{\sim} N(0, \sigma^2). \tag{2}$$

We are interested in $g_1(x_{t-1})$, the smooth of lagged $PM_{2.5}$ . Here we model log-transformed death counts, which can improve normality of residuals.

Confounders to consider:

- Day of the week.
- Seasonality and long-term trends.
- Same-day temperature.
- Same-day dew point temperature.
- Previous day's temperature and dew point temperature.

# Data

```
> load ("NYC.RData")
> str(health)
'data.frame': 1826 obs. of  12 variables:
 $ date      : Date, format: "2001-01-01" "2001-01-02" "2001-01-03" ...
 $ alldeaths : int  171 198 179 169 201 182 167 167 193 159 ...
 $ age65plus : int  122 146 133 128 145 141 126 116 142 124 ...
 $ cardioresp: int  103 106 109 90 120 101 102 101 115 101 ...
 $ cr65plus  : int  90 92 95 77 98 90 88 82 92 88 ...
 $ dow       : chr  "Monday" "Tuesday" "Wednesday" "Thursday" ...
 $ pm25      : num [1:1826, 1] 8.72 13.39 22.9 26.76 25.89 ...
  ..- attr(*, "dimnames")=List of 2
  .. ..$ : chr  "1" "2" "3" "4" ...
  .. ..$ : NULL
 $ Temp      : num  27.6 25.1 25.3 29.8 29.8 33.9 34.9 35.7 32.3 27.6 ...
 $ DpTemp    : num  14.2 11.8 13.1 15.9 20.5 26.7 22.2 31.2 24.4 11.7 ...
 $ rmTemp    : num  27.7 26.8 26 26.7 28.3 ...
 $ rmDpTemp  : num  17.5 14.3 13 13.6 16.5 ...
```

- $DpTemp$ = Dew point temperature.
- $rm$ denotes 3-day running mean of the current day and 2 days prior.
- $dow$ (day of week) is recorded as character.

# Lagged $PM_{2.5}$ Exposure

use default k   need higher k because effects are very non-linear

```
> fit = gam(log(cr65plus)~s(pm25.lag1)+fdow+s(date2, k = 100 )+s(Temp)\\
+ s(DpTemp)+s(rmTemp)+s(rmDpTemp), data = health)
> summary(fit)

Family: gaussian
Link function: identity

Formula:
log(cr65plus) ~ s(pm25.lag1) + fdow + s(date2, k = 100) + s(Temp) +
    s(DpTemp) + s(rmTemp) + s(rmDpTemp)

Parametric coefficients:
                 Estimate Std. Error   t value   Pr(>|t|)
(Intercept)   4.205748765 0.007731497 543.97601 < 2.22e-16 ***
fdowMonday    0.036176289 0.010980266   3.29466  0.0010051 **
fdowSaturday  0.004256722 0.010918397   0.38987  0.6966825
....
---
Signif. codes:  0 ?***? 0.001 ?**? 0.01 ?*? 0.05 ?.? 0.1 ? ? 1
```

# Lagged $PM_{2.5}$ Cont.

approximate F-statistics

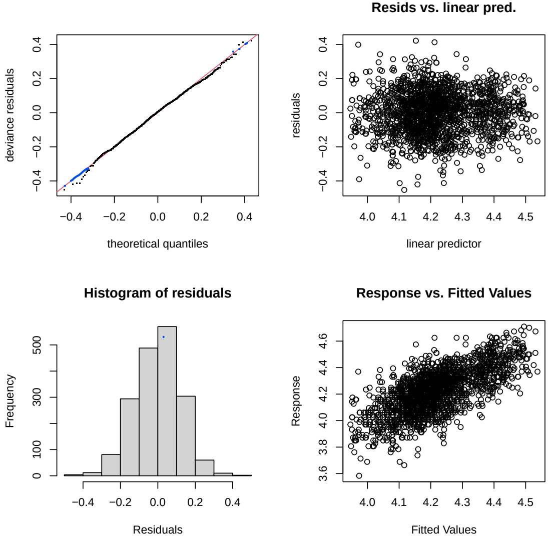
```
Approximate significance of smooth terms:
                   edf    Ref.df        F    p-value
s(pm25.lag1)  1.000040  1.000080  5.50991 0.01902030 *
s(date2)     60.137293 72.669727  6.29239 < 2.22e-16 ***
s(Temp)       1.000002  1.000004 14.33175 0.00015864 ***
s(DpTemp)     1.446148  1.787928  2.05017 0.09521592 .
s(rmTemp)     5.826145  7.051150  2.86630 0.00532417 **
s(rmDpTemp)   1.000004  1.000007  9.45312 0.00214032 **
```

# Diagnostics

```
> gam.check(fit)

Method: GCV   Optimizer: magic
Smoothing parameter selection converged after 17 iterations.
The RMS GCV score gradient at convergence was 3.105686e-08 .
The Hessian was positive definite.
Model rank =  151 / 151

Basis dimension (k) checking results. Low p-value (k-index<1) may
indicate that k is too low, especially if edf is close to k'.

                 k'   edf k-index p-value
s(pm25.lag1)   9.00  1.00    1.04    0.95
s(date2)      99.00 60.14    0.99    0.34
s(Temp)        9.00  1.00    1.00    0.45
s(DpTemp)      9.00  1.45    1.00    0.39
s(rmTemp)      9.00  5.83    1.04    0.94
s(rmDpTemp)    9.00  1.00    1.01    0.69
```

k' > edf, looks good

# Model diagnostics



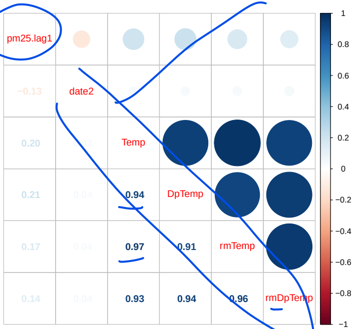
# Correlations and VIF

It is always good to check the correlations between variables.
VIFs are more complicated due to expanding covariates with a spline basis.
Here, we will be concerned if there are high correlations with PM2.5.lag1, which is our variable of scientific interest.

variable of interest

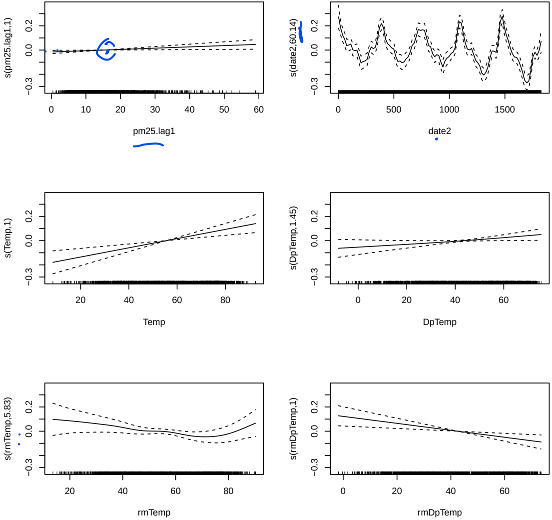
confounders

· high correlations among confounders are not of concern because pm25lag1 is not highly correlated with them



$\sum g(x_i) = 0$
no variability at this pt when shrunk to linear

# Interpretation



ADVANCED:

# Note on time series data

We should analyze the residuals for evidence of autocorrelation.

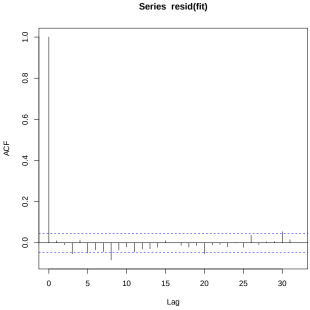
If residuals are correlated, e.g., nearby residuals more similar than distant residuals, inference is not valid, and p-values tend to be too small.

ACF: $corr(\varepsilon_t, \varepsilon_{t-l})$ lag

Recall, we assumed $\varepsilon_t \overset{iid}{\sim} N(0, \sigma^2)$

```
acf(resid(fit))
```

· autocorrelation function




$\pm 1.96 \left(\frac{1}{\sqrt{n}}\right)$

# Interpretation of model

- Daily counts of non-accidental mortality were positively associated with previous-day $PM_{2.5}$ level among those 65 or above.

- Approximately linear on log scale.

```
> newd <- health[1, ] # grab any row
> newd$pm25.lag1 <- 15 - 1e-05 # subtract some small number
> y1 <- predict(fit, newd)
> newd$pm25.lag1 <- 15 + 1e-05 # add some small number
> y2 <- predict(fit, newd)
> (y2 - y1)/2e-05
          1
0.001054248
```

$$\frac{\hat{S}(x_{t_j}+\delta) - \hat{S}(x_{t_j}-\delta)}{2\delta} \approx \hat{S}_j'(x_{t_j}), \text{ here, } \hat{S}_j'(15)$$

$t^{th}$ observation

$j^{th}$ variable

(could do for any $x$...)

- We estimated a 0.00105 increase in log death count per unit ($\mu g/m^3$) increase in $PM_{2.5}$ level in the previous day.

- 10 unit increase in $PM_{2.5}$ level from the previous day increased daily death counts by $100 * (e^{(0.00105\times 10)} - 1)\% = 1.06\%$.

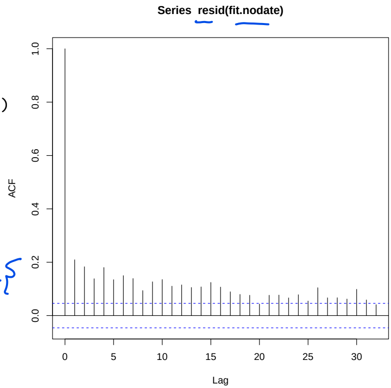
# Example of invalid model

To see the impact of autocorrelation, we remove date.

```
fit.nodate = gam(log(cr65plus)~s(pm25.lag1)
    +fdow+s(Temp)+ s(DpTemp)
    +s(rmTemp)+s(rmDpTemp), data = health)
```

Now, we no longer properly account for the dependence between nearby observations.

This leads to significant autocorrelation $(> 2 * 1/\sqrt{n}))$




- $\hat{\varepsilon}_t$ are not iid

See a lot autocorrelation

$\hat{\beta}_j$s and $\hat{s}_j$s invalid

# Example of invalid model, continued

```
> summary(fit.nodate)

Family: gaussian
Link function: identity

Formula:
log(cr65plus) ~ s(pm25.lag1) + fdow + s(Temp) + s(DpTemp) + s(rmTemp) +
    s(rmDpTemp)

Parametric coefficients:
               Estimate Std. Error t value Pr(>|t|)
(Intercept)   4.2196867  0.0086125 489.950   <2e-16 ***
fdowFriday   -0.0149662  0.0121799  -1.229   0.2193
...

Approximate significance of smooth terms:
               edf Ref.df      F p-value
s(pm25.lag1) 1.000  1.000 47.599  <2e-16 ***
s(Temp)      1.683  2.177  4.480  0.0103 *
s(DpTemp)    1.000  1.000  1.406  0.2359
s(rmTemp)    7.705  8.572  6.781  <2e-16 ***
s(rmDpTemp)  2.111  2.762  1.906  0.1233
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

R-sq.(adj) =  0.337   Deviance explained = 34.4%
GCV = 0.019388  Scale est. = 0.01917   n = 1825
```

very significant, but probably too small because of violations of independence of residuals.
· Need to use model with s(date)

# Autocorrelation in residuals

One person's mean structure is another person's correlation structure.

If you don't have covariates to model the correlation structure, you can specify correlated errors.

This is beyond the scope of this course, but a nice tutorial is available at https://petolau.github.io/Analyzing-double-seasonal-time-series-with-GAM-in-R/

# Bivariate Splines

# Bivariate Splines

Under an additive model framework, we can also consider smooth effects of two variables jointly:

$$y_i = f(x_i, z_i) + \varepsilon_i$$

We can think of $f(x_i, z_i)$ as a surface.

We can use 2-dimensional splines to model $f(x_i, z_i)$.

Let $\mathbf{s}_i = (x_i, z_i)$ be some pair of covariate values, and let $\mathbf{k}_m = (x_m, z_m)$ denote the $m^{\text{th}}$ knot in the domain of $x_i$ and $z_i$. We can express the smooth function as

$$f(x_i, z_i) = \beta_0 + \sum_{m=1}^{M} \beta_m b_m(\underset{(x_i, z_i)}{\tilde{s}_i}, \underset{(x_m, z_m)}{\tilde{k}_m})$$

Note that $b_m( \;,\; )$ is a basis function that maps $\mathbb{R} \times \mathbb{R} \to \mathbb{R}$.

# Thin-plate Spline

One popular bivariate basis function uses thin-plate splines, which extends to $\mathbf{s}_i \in \mathbb{R}^d$ and $\partial^l g$ penalties. We consider $d = 2$ and $l = 2$:

$$f(\tilde{s}_i) = \beta_0 + \beta_1 x_t + \beta_2 z_t + \sum_{m=1}^{M} \beta_{2+m} b_m(\tilde{s}_i ; \tilde{k}_m)$$

using the radial basis:

$$b_m(\tilde{s}_i, \tilde{k}_m) = ||\tilde{s}_i - \tilde{k}_m||^2 \log ||\tilde{s}_i - \tilde{k}_m||$$

Here, $||\mathbf{s}_i - \mathbf{k}_m||$ is the Euclidean distance between the covariate $\mathbf{s}_i$ and the knot location $\mathbf{k}_m$.

The radial basis kernel is $r^2 \log r$.

The thin-plate spline is sensitive to the scale of each variable, but invariant to rotation (isotropic).

It is best for variables measured on the same scale (e.g. geographical distance).

# Thin-plate Spline, cont.

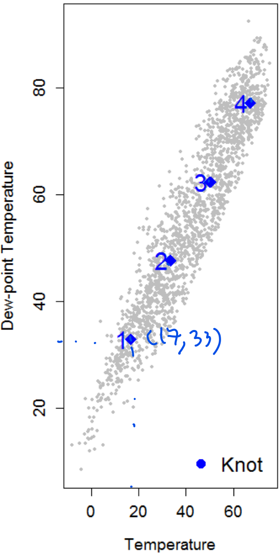
It can be shown that the thin-plate spline function minimizes

$$\sum_{i=1}^{n}\{y_i - f(x_i, z_i)\}^2$$
$$+ \lambda \int \left(\frac{\partial^2 f(x,z)}{\partial x^2}\right)^2 + 2\left(\frac{\partial^2 f(x,z)}{\partial x\,\partial z}\right)^2 + \left(\frac{\partial^2 f(x,z)}{\partial z^2}\right)^2 \, dxdz \ .$$

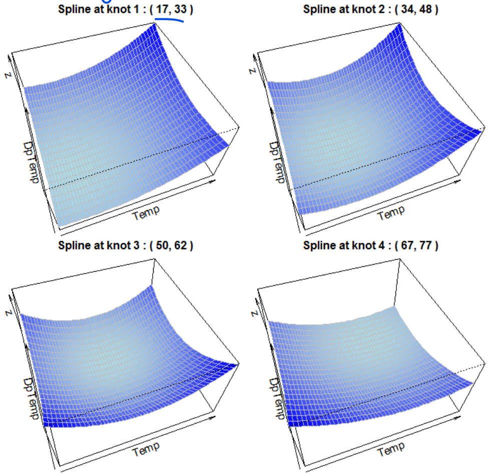
More information is in Wood 2017, pages 215-221, and references therein.

intuition: second derivatives measure wiggliness,
penalize second derivative

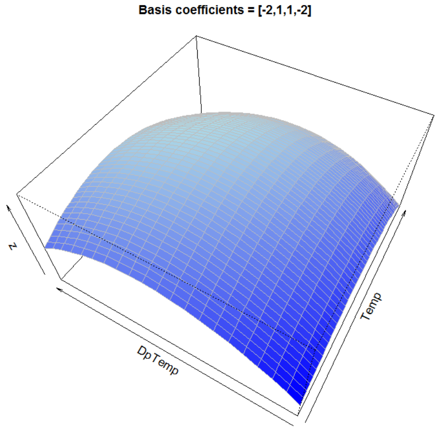
# Thin-plate Spline

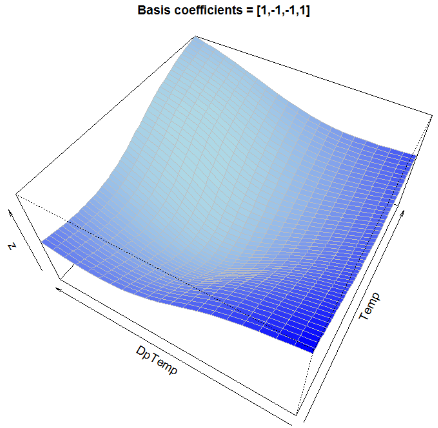



$z = r^2 \log r$



# Thin-plate Spline



# Thin-plate regression spline

mgcv::gam uses thin-plate regression splines as the default for smoothers of a single variable (as well as two variables).

This is implemented in a 'knot-free' manner.
This is the general idea.
For $d = 2$, $l = 2$:

1. Construct the $n \times n$ matrix $\mathbf{E}$ from $||\mathbf{s}_i - \mathbf{s}_{i'}||^2 \log(||\mathbf{s}_i - \mathbf{s}_{i'}||)$.
2. Use the singular value decomposition to find a low rank representation, e.g., $k$ leading singular vectors, and use this in place of $\mathbf{X}$ in the penalized objective function.
3. In practice, there are some additional things to worry about to make $\mathbf{1}$ (for the intercept), $\boldsymbol{x}$ and $\boldsymbol{z}$ in the null space of the penalty.
4. Then estimate the $\beta_0$, $\beta_1$ for $\boldsymbol{x}$, $\beta_2$ for $\boldsymbol{z}$ (unpenalized) and $\beta_3, \ldots, \beta_k$ (penalized), which dramatically reduces computation costs.

The formulas for the general case ($d$ dimensions and $l$th derivative) get a bit complicated; see 5.5 in Wood.

# Joint Effects of Temperature and Dew point Temperature

To define a bivariate smoother, simply specify $s(var_1, var_2)$ in the equation formula.

Default in `mgcv:gam` is to use a thin-plate regression spline.

For this demonstration, let's look at the joint effects of same-day temperature and dew point temperature on log mortality, controlling only for time trends.

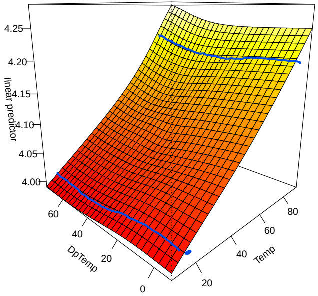
specifies bivariate smooth

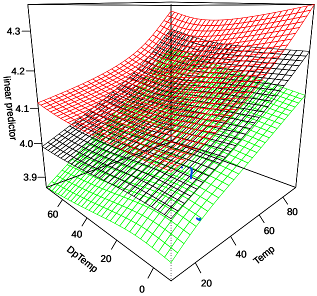
```
> fit1 = gam(log(alldeaths)~s(date2, k=100) + s(Temp, DpTemp, k = 20), data = health)
> summary (fit1)

Parametric coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 4.219108   0.002953    1429   <2e-16 ***

Approximate significance of smooth terms:
                  edf Ref.df     F  p-value
s(date2)       69.527 82.144 8.501  < 2e-16 ***
s(Temp,DpTemp)  5.938  8.032 6.407 2.96e-08 ***

R-sq.(adj) =   0.45   Deviance explained = 47.3%
GCV score = 0.016624  Scale est. = 0.015928  n = 1826
```

You should also use `gam.check` (note shown here)

# Joint Effects of Temperature and Dew Point Temperature

## Perspective Plots from Thin-Plate Spline




red/green are +/− 2 s.e.

SKIPPED

· Direct extension of interactions between univariate smooths

# Tensor Product

Another way to obtain a 2-D spline is by construction. First consider the effect of a variable $x_i$ specified by $M$ basis functions $b_m(x_i)$

$$f(x_i) = \sum_{m=0}^{M} \beta_m b_{m,x}(x_i).$$

Now assume $f(x_i, z_i)$ is created by allowing each spline coefficient to vary with the second variable $z_i$:

$$f(x_i, z_i) = \sum_{m=0}^{M} \beta_m(z_i) b_{m,x}(x_i).$$

We can express $\beta_m(z_i)$ also as a smooth function of $z_i$ using $N$ basis functions $b_{n,z}(z_i)$:

$$f(x_i, z_i) = \sum_{m=0}^{M} \sum_{n=0}^{N} \alpha_{m,n} b_{n,z}(z_i) b_{m,x}(x_i).$$

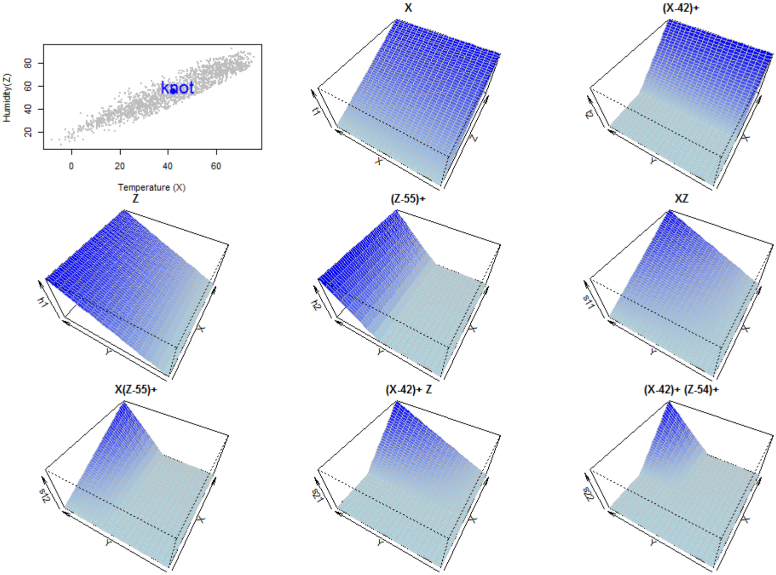
This is equivalent to expressing $f(x_i, z_i)$ as all pairwise basis functions of $x_i$ and $z_i$:

$$f(x_i, z_i) = \sum_{m=0}^{M} \sum_{n=0}^{N} \alpha_{m,n} b_{n,z}(z_i) b_{m,x}(x_i).$$

# Tensor Product

Example with 1 knot: write out all pairwise interactions

# Tensor Product Example



# Tensor Product

The roughness penalty optimized by the tensor product is

$$\sum_{i=1}^{n}\{y_i - f(x_i, z_i)\}^2 + \int \lambda_x \left(\frac{\partial^2 f(x,z)}{\partial x^2}\right)^2 + \lambda_z \left(\frac{\partial^2 f(x,z)}{\partial z^2}\right)^2 \, dxdz \, .$$

- Allows penalization in each variable dimension by assigning a smoothing parameter for each marginal smooth effect.
- Choice of basis function and knots also do not need to be the same for each covariate.
- Provides a recipe for constructing flexible multivariate joint effects.
- Often used for modeling interactions where the degree of smoothness may not be the same for all covariates.

# Fitting Tensor Product

A bivariate smoother using tensor product is specified by `te( var_1, var_2, bs=‘‘cr’’)` in the equation formula.

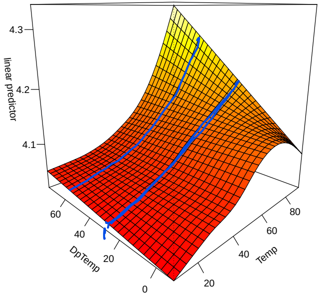
Recommended when scales differ.

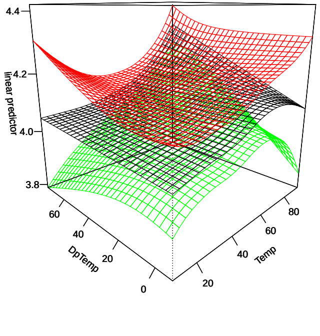
The option `bs = ‘‘cr’’` specifies using cubic spline functions for each covariate .

```
> fit1 = gam (log(alldeaths) ~ s(date2, k = 100) +
        te(Temp, DpTemp, k = 20, bs = "cr") , data = health)

> summary (fit1)

Parametric coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 4.219108   0.002952    1429   <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(date2)        68.353 81.039  8.343  <2e-16 ***
te(Temp,DpTemp)  6.003  7.391 18.134  <2e-16 ***

R-sq.(adj) =   0.45   Deviance explained = 47.3%
GCV score = 0.016601  Scale est. = 0.015916  n = 1826
```

# Joint Effects of Temperature and Dew Point Temperature

Perspective Plots from Cubic Tensor Product Spline



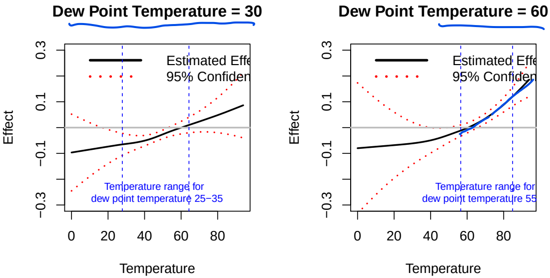



* covered

# Marginal Effects

By fitting an effect surface, we can obtain slices with respect to a covariate and examine the conditional effect of another covariate.

For example, we can look at the non-linear effect of temperature when dew point temperature = 30 versus 60.




small modification of the effect temperature by dew point temperature

# $PM_{2.5}$ and Temperature

Let's revisit the $PM_{2.5}$ analysis. An important research question is whether there is an interaction between air pollution and temperature.

For this demonstration, we consider previous-day $PM_{2.5}$ level and 3-day moving average of temperature (rmTemp).

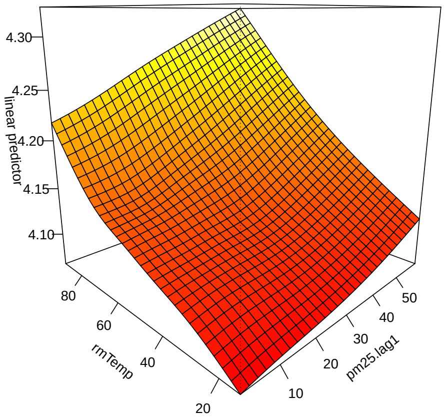
We use thin-plate splines, which are much faster to fit than tensor; pm25.lag1 and rmTemp are very roughly on same scale.

# Bivariate smooth for rmTemp and PM2.5

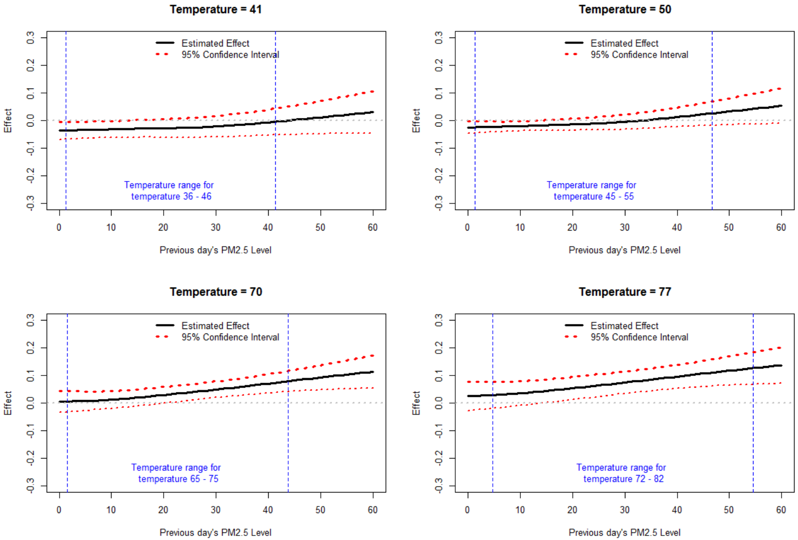
```
> fit = gam(log(alldeaths)~s(pm25.lag1, rmTemp)+factor(dow)+s(date2, k = 75)+
                            s(DpTemp)+s(rmDpTemp), data = health)
> summary (fit)

Parametric coefficients:
                      Estimate Std. Error t value Pr(>|t|)
(Intercept)          4.2191876  0.0077934 541.380   <2e-16 ***
factor(dow)Friday   -0.0142658  0.0110132  -1.295   0.1954
factor(dow)Monday    0.0222996  0.0110146   2.025   0.0431 *
factor(dow)Saturday -0.0092121  0.0110082  -0.837   0.4028
factor(dow)Thursday  0.0011288  0.0110248   0.102   0.9185

Approximate significance of smooth terms:
                      edf Ref.df      F  p-value
s(pm25.lag1,rmTemp)  5.858  8.381  4.048 6.35e-05 ***
s(date2)            57.808 66.508  6.721  < 2e-16 ***
s(DpTemp)            1.362  1.633 25.075 8.11e-10 ***
s(rmDpTemp)          1.000  1.000 35.085 3.79e-09 ***

R-sq.(adj) =  0.456   Deviance explained = 47.8%
GCV score = 0.016379  Scale est. = 0.015724  n = 1825
```

# Bivariate smooth for rmTemp and $PM_{2.5}$

Effect of temperature is more pronounced than $PM_{2.5}$.



# PM$_{2.5}$ Effect Modification by Temperature?



# Extracting Effects from Smooth Function

- Let's say we are interested in the difference in $f(x_i)$ when $x_i$ increases from value $a$ to value $b$:
  E.g., (40,70) to (50,70)

$$\hat{f}(b) - \hat{f}(a) = \sum_{m=1}^{M} \hat{\beta}_m b_m(b) - \sum_{m=1}^{M} \hat{\beta}_m b_m(a) = \sum_{m=1}^{M} \hat{\beta}_m \{b_m(b) - b_m(a)\}.$$

The covariance matrix is given by
$Cov(\mathbf{B}'_{b-a}\hat{\boldsymbol{\beta}}) = B'_{b-a} Cov(\hat{\beta}) B_{b-a}$ , where

$$B_{b-a} = [b_1(b) - b_1(a), \ldots, b_M(b) - b_M(a)]$$

- However $b_m()$'s are basis functions and $b_m(b) - b_m(a) \neq b_m(b-a)$. We will need to construct the new covariate vector **B** ourselves.

# Extracting Effects from a Smooth Function

We want to estimate the effect of a 10 $\mu g/m^3$ increase in $PM_{2.5}$ levels from 40 to 50 $\mu g/m^3$ when temperature = 70F.

```
> X1 = predict(fit, data.frame(pm25.lag1 = 40, rmTemp=70,
+            DpTemp=0, rmDpTemp = 0, dow = "Sunday", date2=0),type= "lpmatrix")
> X2 = predict(fit, data.frame(pm25.lag1 = 50, rmTemp=70,
+            DpTemp=0, rmDpTemp = 0, dow = "Sunday", date2=0),type= "lpmatrix")

> X.diff = X2 - X1
> dim (X.diff)
[1]   1 128
> Est = X.diff %*% coef (fit)  ## Estimate
> se = sqrt( X.diff %*% vcov (fit) %*% t(X.diff) ) ## Standard Error
> Est; se
        [,1]
1 0.02213508
           1
1 0.01096592
```

$B_b$ from previous slide along with other variables

combine variances and covariances

So our estimate is 0.022 (95%CI 0.001, 0.044).

The same effect of a 10-unit increase in $PM_{2.5}$ levels from 20 to 30 $\mu g/m^3$ is 0.020 (95%CI 0.004, 0.036).

These two estimates are very similar because the $PM_{2.5}$ effect appears to be quite linear.

# Inference in models with smoothing splines

For parametric terms, the inference is identical to purely parametric model.

You can use the t-statistics from `summary(fit)`.

```
> fit.full = gam(log(cr65plus)~s(pm25.lag1, rmTemp)+fdow+s(date2, k = 100)+s(DpTemp)+s(rmDp
> summary(fit.full)

Family: gaussian
Link function: identity

Formula:
log(cr65plus) ~ s(pm25.lag1, rmTemp) + fdow + s(date2, k = 100) +
    s(DpTemp) + s(rmDpTemp)

Parametric coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept)    4.219093   0.007784 541.997   <2e-16 ***
fdowFriday    -0.014166   0.011001  -1.288   0.1980
fdowMonday     0.022352   0.011002   2.032   0.0423 *
fdowSaturday  -0.009111   0.010995  -0.829   0.4074
fdowThursday   0.001261   0.011012   0.114   0.9089
fdowTuesday   -0.001689   0.011002  -0.153   0.8780
fdowWednesday  0.000470   0.011012   0.043   0.9660
---
Signif. codes:  0 ?***? 0.001 ?**? 0.01 ?*? 0.05 ?.? 0.1 ? ? 1
```

all the usual SEs (no change from lm)

can test significance of fdow with anova

# Inference in models with smoothing splines

For overall effect of `fdow`, use `anova`:

```
> anova(fit.full)

Family: gaussian
Link function: identity

Formula:
log(cr65plus) ~ s(pm25.lag1, rmTemp) + fdow + s(date2, k = 100) +
    s(DpTemp) + s(rmDpTemp)

Parametric Terms:
     df     F p-value
fdow  6 2.154  0.0448
```

# Inference in models with smoothing splines

For smoothed terms, the inference is approximate because the distribution of the test statistics is impacted by the penalization.

The idea is to jointly test the significance of the $\hat{\beta}_j$ for the coefficients corresponding to the spline of the $j$th smooth term.

There is some discussion of these approximate p-values in `?summary.gam`. For detailed discussion, see Wood 2017 p.304.

Approximate inference for smooth effects:

```
Approximate significance of smooth terms:
                      edf Ref.df      F  p-value    
s(pm25.lag1,rmTemp)  5.433  7.738  4.246 6.30e-05 ***
s(date2)            62.047 74.627  6.118  < 2e-16 ***
s(DpTemp)            1.210  1.379 29.260 2.89e-09 ***
s(rmDpTemp)          1.000  1.000 34.655 4.68e-09 ***

R-sq.(adj) =  0.458   Deviance explained =   48%
GCV = 0.016377  Scale est. = 0.015688  n = 1825
```

# Inference in models with smoothing splines

Should we use a bivariate spline for pm25.lag1 and rmTemp, or two univariate splines? Don't do this:

fits two univariate smooths for pm25.lag1 and rmTemp

```
> anova(fit.reduced2,fit.full,test='F')
Analysis of Deviance Table

Model 1: log(cr65plus) ~ s(pm25.lag1) + s(rmTemp) + s(date2, k = 100) +
    fdow + s(DpTemp) + s(rmDpTemp)
Model 2: log(cr65plus) ~ s(pm25.lag1, rmTemp) + fdow + s(date2, k = 100) +
    s(DpTemp) + s(rmDpTemp)
  Resid. Df Resid. Dev        Df     Deviance F Pr(>F)
1 1734.9095  27.353616
2 1733.2552  27.428321 1.6542684 -0.074705162
```

Note: HW was different we had an "interaction" between a continuous variable and categorical variable; here, we are looking at 2 continuous variables

What happened here?

Models are not nested.

Using tensor splines, we can construct in a special way to make nested. Then we can recast the problem as testing for an interaction.

# Testing for an interaction

To test for an interaction between pm25.lag1 and rmTemp, we can construct the tensor spline in a special way such that the univariate splines are in the null space of the penalty of the tensor spline. See pages 243 and the example on page 343-346.

```
fit.full.tensor = gam(log(cr65plus)~s(pm25.lag1,bs='cr')+s(rmTemp,bs='cr')
+ti(pm25.lag1, rmTemp,bs='cr')+fdow+s(date2, k = 100)+s(DpTemp)+s(rmDpTemp), data = health)
summary(fit.full.tensor)
anova(fit.full.tensor)
```

# Testing for an interaction

```
> anova(fit.full.tensor)

Family: gaussian
Link function: identity

Formula:
log(cr65plus) ~ s(pm25.lag1, bs = "cr") + s(rmTemp, bs = "cr") +
    ti(pm25.lag1, rmTemp, bs = "cr") + fdow + s(date2, k = 100) +
    s(DpTemp) + s(rmDpTemp)

Parametric Terms:
     df    F p-value
fdow  6 2.24  0.0371

Approximate significance of smooth terms:
                        edf Ref.df      F p-value
s(pm25.lag1)          1.000  1.001  4.147  0.0418
s(rmTemp)             5.301  6.480  2.524  0.0171
ti(pm25.lag1,rmTemp)  1.000  1.000  3.463  0.0629
s(date2)             59.917 72.436  6.143  <2e-16
s(DpTemp)             1.000  1.000 41.860  <2e-16
s(rmDpTemp)           1.000  1.000 31.651  <2e-16
```

$H_0$: $f_{xz}(x_i, z_i)$ does not improve model fit over $f_x(x_i)$ and $f_z(z_i)$.
p=0.06, 0.06 > 0.05, $f_{xz}$ does not significantly improve model fit

# Inference in models with smoothing splines

Let's refit the model with pm25.lag1 as a linear term.

```
> fit.reduced3 = gam(log(cr65plus)~pm25.lag1+s(rmTemp)

+s(date2, k = 100)+fdow+s(DpTemp)+s(rmDpTemp), data = health)
> summary(fit.reduced3)

Family: gaussian
Link function: identity

Formula:
log(cr65plus) ~ pm25.lag1 + s(rmTemp) + s(date2, k = 100) + fdow +
    s(DpTemp) + s(rmDpTemp)

Parametric coefficients:
                Estimate Std. Error t value Pr(>|t|)
(Intercept)    4.203e+00  1.018e-02 412.689   <2e-16 ***
pm25.lag1      1.073e-03  4.508e-04   2.381   0.0174 *
fdowFriday    -1.478e-02  1.099e-02  -1.345   0.1789
fdowMonday     2.249e-02  1.098e-02   2.048   0.0407 *
fdowSaturday  -9.026e-03  1.098e-02  -0.822   0.4110
fdowThursday   5.425e-04  1.100e-02   0.049   0.9607
fdowTuesday   -1.433e-03  1.098e-02  -0.130   0.8962
fdowWednesday  9.336e-05  1.100e-02   0.008   0.9932
...
R-sq.(adj) =  0.459   Deviance explained = 48.2%
GCV = 0.016324  Scale est. = 0.015642  n = 1825
```

"Reduced"

# GAM or linear?

It may seem like we can test for whether or not to include a smooth term versus linear term using anova. However, the anova test can produce funny results when the EDF is approximately one, as the change in DF is very small. So, I suggest not doing this:

```
> anova(fit.reduced2,fit.reduced3,test='F')
Analysis of Deviance Table

Model 1: log(cr65plus) ~ s(pm25.lag1) + s(rmTemp) + s(date2, k = 100) +
    fdow + s(DpTemp) + s(rmDpTemp)
Model 2: log(cr65plus) ~ pm25.lag1 + s(rmTemp) + s(date2, k = 100) + fdow +
    s(DpTemp) + s(rmDpTemp)
  Resid. Df Resid. Dev       Df   Deviance      F Pr(>F)
1    1734.9     27.354
2    1734.9     27.353 0.016157 0.00029882 1.1824 0.0325 *
---
Signif. codes:  0 ?***? 0.001 ?**? 0.01 ?*? 0.05 ?.? 0.1 ? ? 1
```

df are tiny, weird things can happen

# GAM or linear?

When you have an effect that is close to linear, your interpretation is very similar whether or not you use a gam, and when EDF=1, then the approximate p values are equivalent to refitting with a linear term.

To determine whether or not to include a smooth or linear effect, I suggest looking at the EDF. If it is greater than 1, than it seems reasonable to use a smooth term.

There is not really any disadvantage to modeling with a smooth term, except for some extra work we need to do for interpretation.

One approach to test for a non-linear effect is to construct a special spline that separates the linear and non-linear parts:
https://stats.stackexchange.com/questions/449641/is-there-a-hypothesis-test-that-tells-us-whether-we-should-use-