Generalized additive (mixed) models

```
library(mgcv)
library(gratia)
library(tidyverse)
```

Additive models

- generally a way to specify more complex (smooth) terms based on *individual* covariates: $\mu = \beta_0 + f_1(x_1) + f_2(x_2) + \ldots$
- lots of ways to generate $f_i(x_i)$: kernel estimators, locally weighted polynomials, … see T. J. Hastie and Tibshirani (1990), T. Hastie, Tibshirani, and Friedman (2009) (*backfitting algorithm* etc.)
- we will focus on

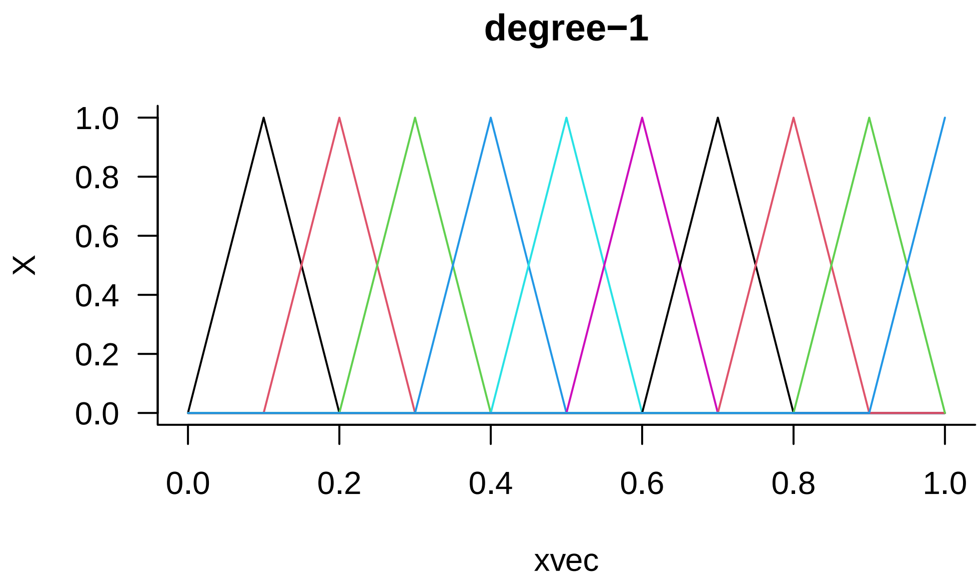
Basis expansions

- (theoretically) infinitely expandable
- e.g. polynomials ('regular'/raw, orthogonal, Legendre, Hermite)
- wavelet, Fourier
- splines: **piecewise polynomial** with continuity/smoothness constraints

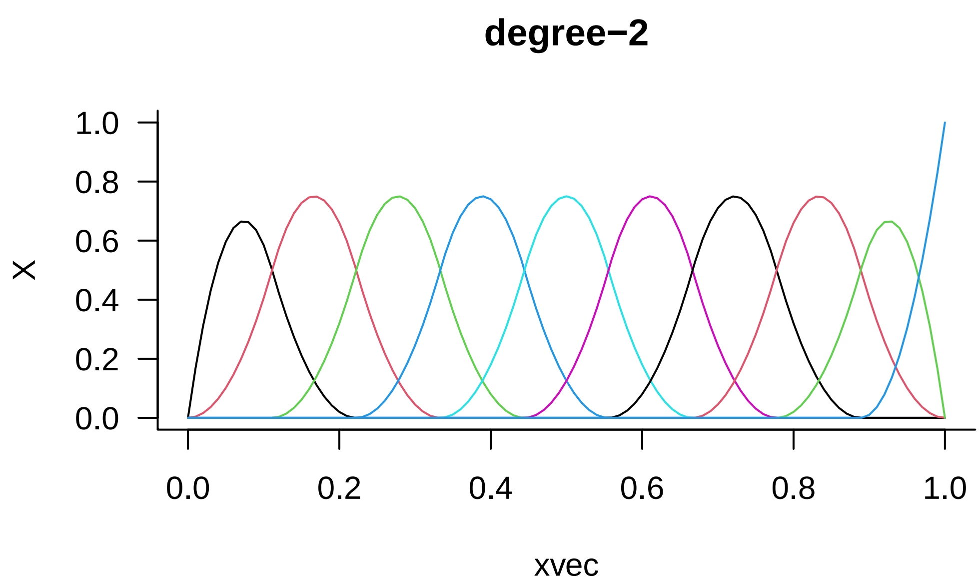
Spline degree

```
xvec <- seq(0, 1, length.out = 101)
sfun <- function(d = 3, type = "bs", ...) {
    if (type == "bs") {
        X <- splines::bs(xvec, df = 10, degree = d)
    } else {
        X <- splines::ns(xvec, df = 10)
```

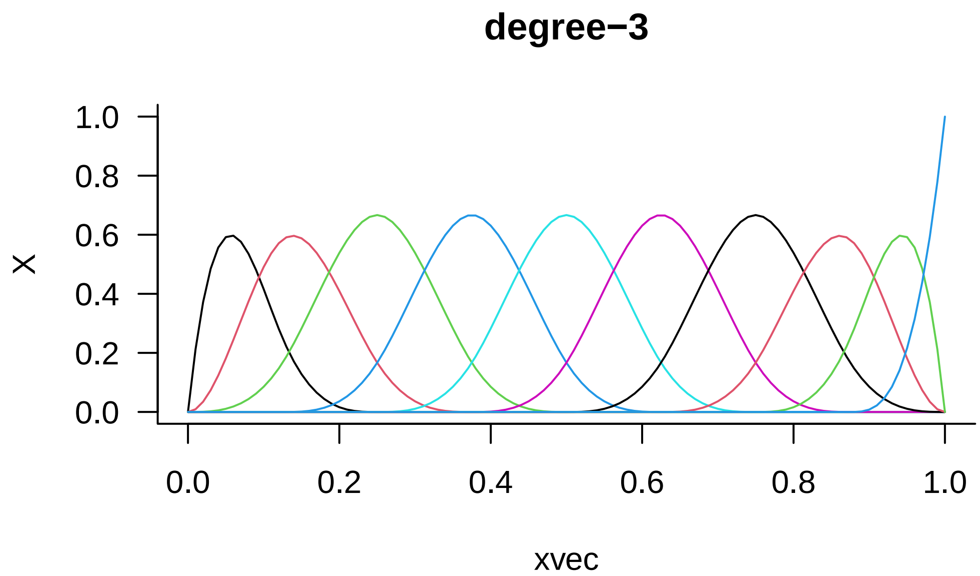
```r
    }
    par(bty = "l", las = 1)
    matplot(xvec, X, type = "l", lty = 1, ...)
}
sfun(d = 1, main = "degree-1")
```




```r
sfun(d = 2, main = "degree-2")
```



```r
sfun(d = 3, main = "degree-3")
```



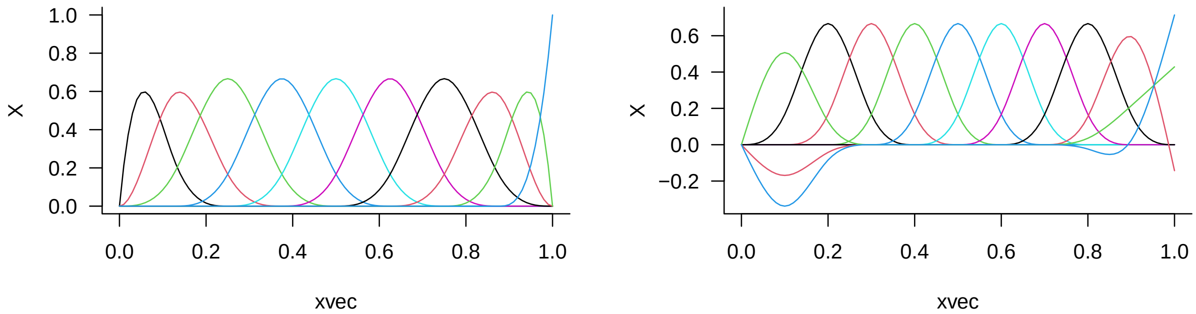
spline terminology

- **knots**: breakpoints (boundary, interior)
- order-M (ESL): continuous derivatives up to order $M-2$ (cubic, $M=4$)
- typically $M = 1$, 2, 4
- number of knots = df (degrees of freedom) -1 -intercept

Spline choices

- continuous derivatives up to $d-1$
- truncated polynomial basis (simple)
- B-splines: complex, but *minimal support*/maximum sparsity
- *natural* splines: extra constraint, derivatives > 1 vanish at boundaries

```r
par(mfrow = c(1,2))
sfun()
sfun(type = "ns")
```



choosing knot locations

- generally not that important: evenly spaced, *or* evenly spaced based on quantiles

choosing basis dimension

- in principle could expand dimension to match total number of points (*interpolation spline*)
- … but that would overfit
- AIC, adjusted R^2, cross-validation …

smoothing splines

- as many knots as data points
- plus squared-second-derivative ("wiggliness") penalty

$$\text{RSS} + \lambda \int (f''(t))^2 \, dt$$

- defined on an infinite-dimensional space
- minimizer is a natural cubic spline with knots at x_i

$$(\mathbf{y} - \mathbf{Z}\mathbf{b})^\top (\mathbf{y} - \mathbf{Z}\mathbf{b}) + \lambda \mathbf{b}^\top \Omega \mathbf{b}$$

with $\{\Omega\}_{jk} = \int \mathbf{Z}_j''(t)\mathbf{Z}_k''(t)\, dt$ $$

- **generalized** ridge regression: penalize by $\lambda\Omega_N$ rather than λI
- same data augmentation methods as before except that now we use $\sqrt{\lambda}C$ where C is a matrix, and the "square root" (Cholesky factor) of Ω_N

See Simon N. Wood (2017), Perperoglou et al. (2019)

connection to mixed models

- note that $\lambda \mathbf{b}^\top \Omega \mathbf{b}$ is equivalent to $(1/\sigma^2)\mathbf{b}\Sigma'^{-1}\mathbf{b}^\top$; if Σ' is a *scaled* covariance matrix (i.e. $\Sigma = \sigma^2\Sigma$), then this is the core of the MVN log-likelihood $\log L(\mathbf{b}|\Sigma)$ (all we're missing is a factor of $\text{Det}(\Sigma)^{-1/2}$ and a normalization constant)
- So we can fit this with any of the mixed model machinery, provided we can set up the correct covariance matrix
- Or

generalized cross-validation score

- very close to AIC
- Larsen (2015), Golub, Heath, and Wahba (1979)
- minimize $\text{RSS}/(\text{Tr}(\mathbf{I}-\mathbf{S}(\lambda)))^2$, where S is
- "a rotation-invariant version of PRESS" $(\sum(e_i/(1-h_i i))^2)$
- replace RSS with approximation of deviance,

$$||\sqrt{\mathbf{W}}(\mathbf{z}-\mathbf{X}\beta)||^2$$

  for generalized (non-Gaussian) models

ML criterion, REML criterion

- treat spline smoothing as a *mixed model* problem
- spline (penalized) parameters are $\mathbf{u}$
- $y|u \sim N(\mathbf{X}\beta + \mathbf{Zu}, \sigma^2\mathbf{I})$; $\mathbf{u} \sim N(0, (\sigma^2/\lambda)\mathbf{W}^{-1})$
- where the $\mathbf{W}$ is the penalty matrix
- corresponds to minimizing $||\mathbf{y}-\mathbf{X}\beta-\mathbf{Zu}||^2 + \lambda\mathbf{u}^\top\mathbf{Wu}$
- "fixed effects are viewed as random effects with improper uniform priors and are integrated out" (Wood 2011)
- Laplace approximation

practical stuff

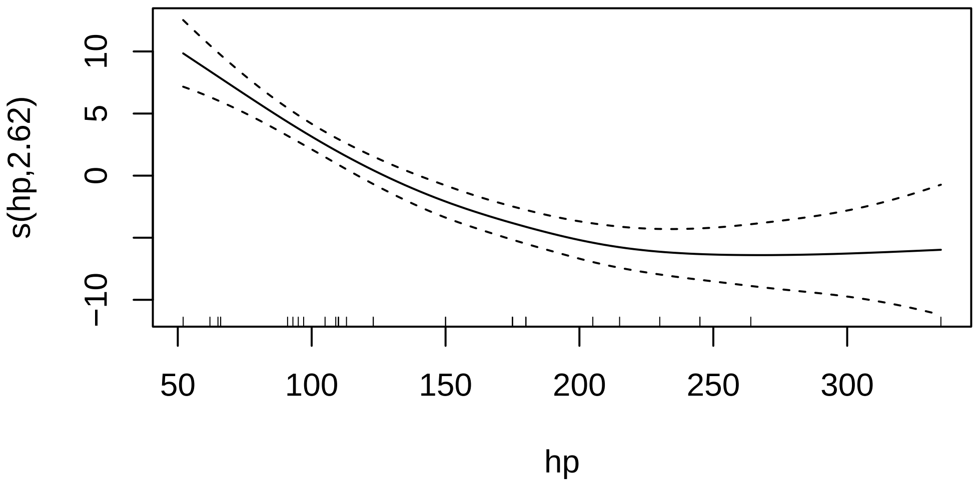
- Simon Wood is insanely smart, and `mgcv` is insanely powerful and flexible
- gratia package (named after Grace Wahba
- available 'smooths' (bases + penalty terms): look for strings of the form `smooth.construct.*.smooth.spe`
- although you can *theoretically* have as many knots as data points, fewer is often good enough/computationally efficient

```
 [1] "ad"     "bs"     "cc"     "cp"     "cr"     "cs"     "ds"     "gp"
 [9] "mrf"    "ps"     "re"     "sf"     "so"     "sos"    "sw"     "t2"
[17] "tensor" "tp"     "ts"
```

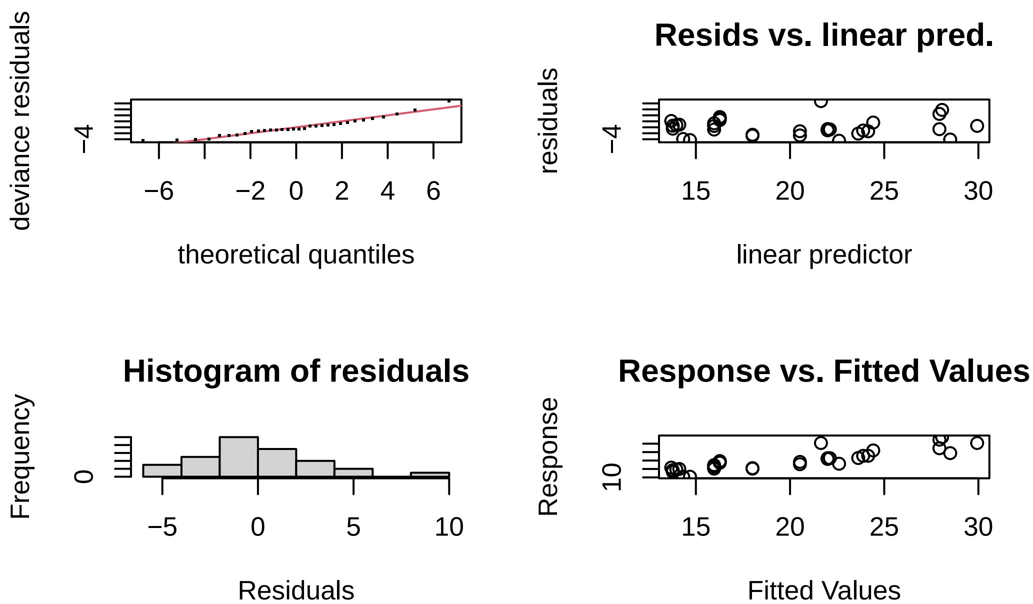
```r
g1 <- gam(mpg ~ s(hp), data = mtcars)
summary(g1)
```

```
Family: gaussian
Link function: identity

Formula:
mpg ~ s(hp)

Parametric coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  20.0906     0.5487   36.62   <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(hp) 2.618  3.263 26.26  <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

R-sq.(adj) =  0.735   Deviance explained = 75.7%
GCV = 10.862  Scale est. = 9.6335    n = 32
```

```r
plot(g1)
```



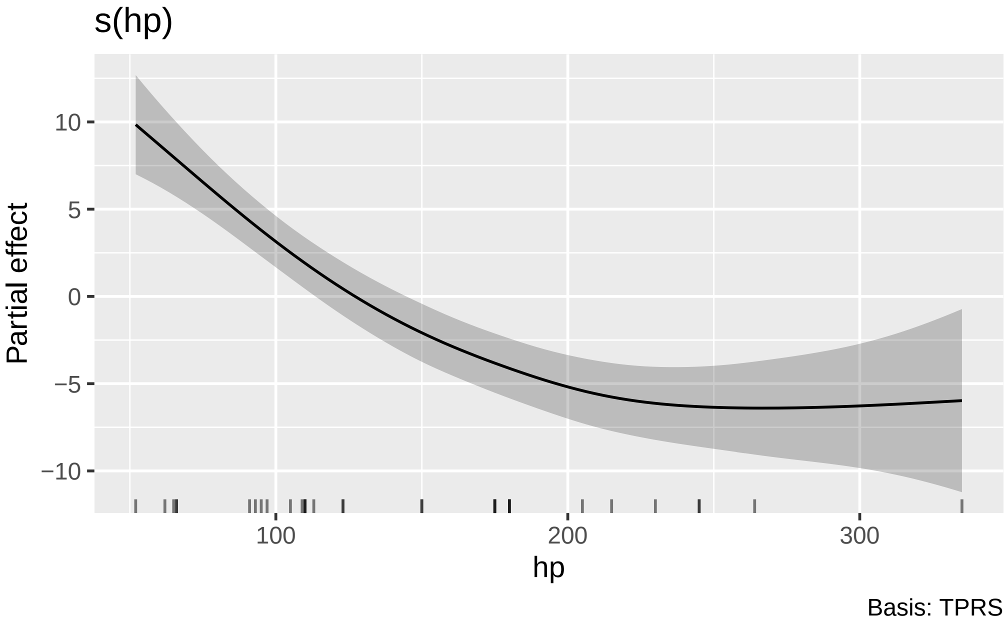

```
gam.check(g1)
```



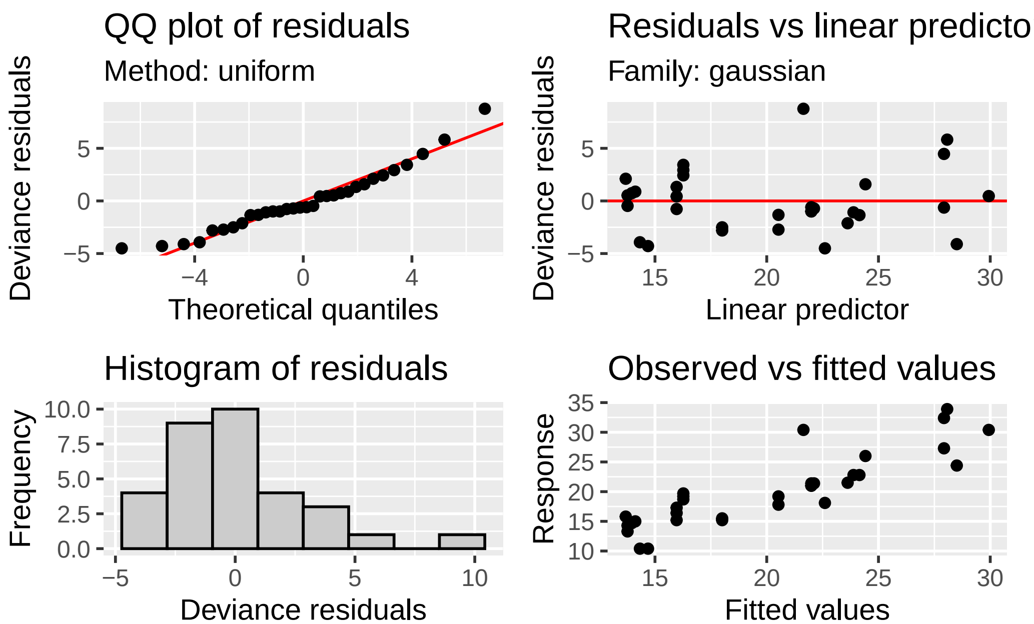

```
Method: GCV   Optimizer: magic
Smoothing parameter selection converged after 4 iterations.
The RMS GCV score gradient at convergence was 4.290111e-05 .
The Hessian was positive definite.
Model rank =  10 / 10
```

```
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(hp) 9.00 2.62    0.87     0.2
```

```r
draw(g1)
```



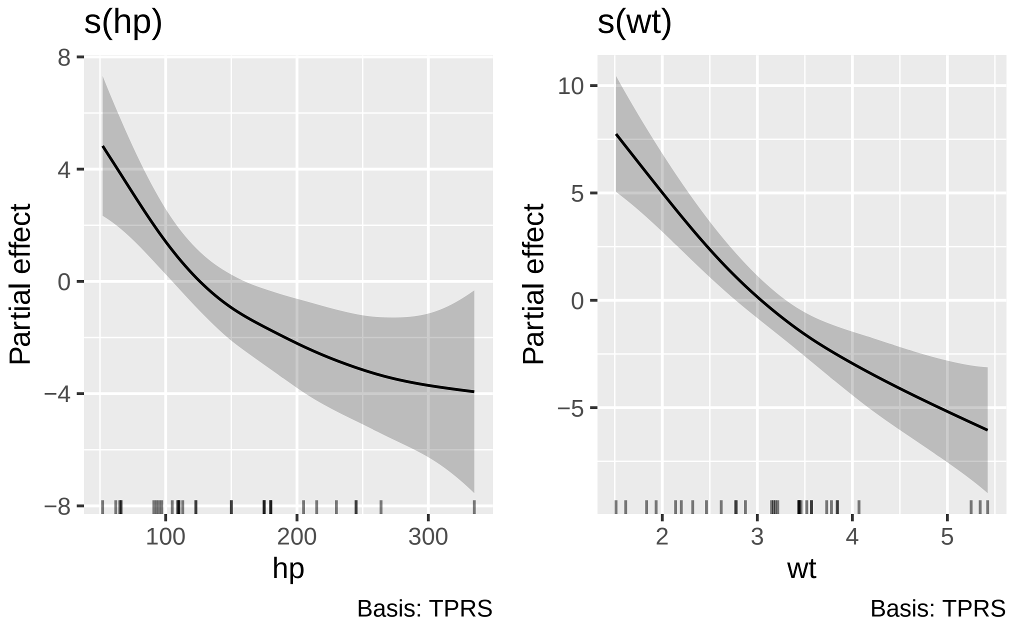

```r
appraise(g1)
```




```
g2 <- gam(mpg ~ s(hp), data = mtcars, fit = FALSE)
```

concurvity: CV question, Ramsay, Burnett, and Krewski (2003)

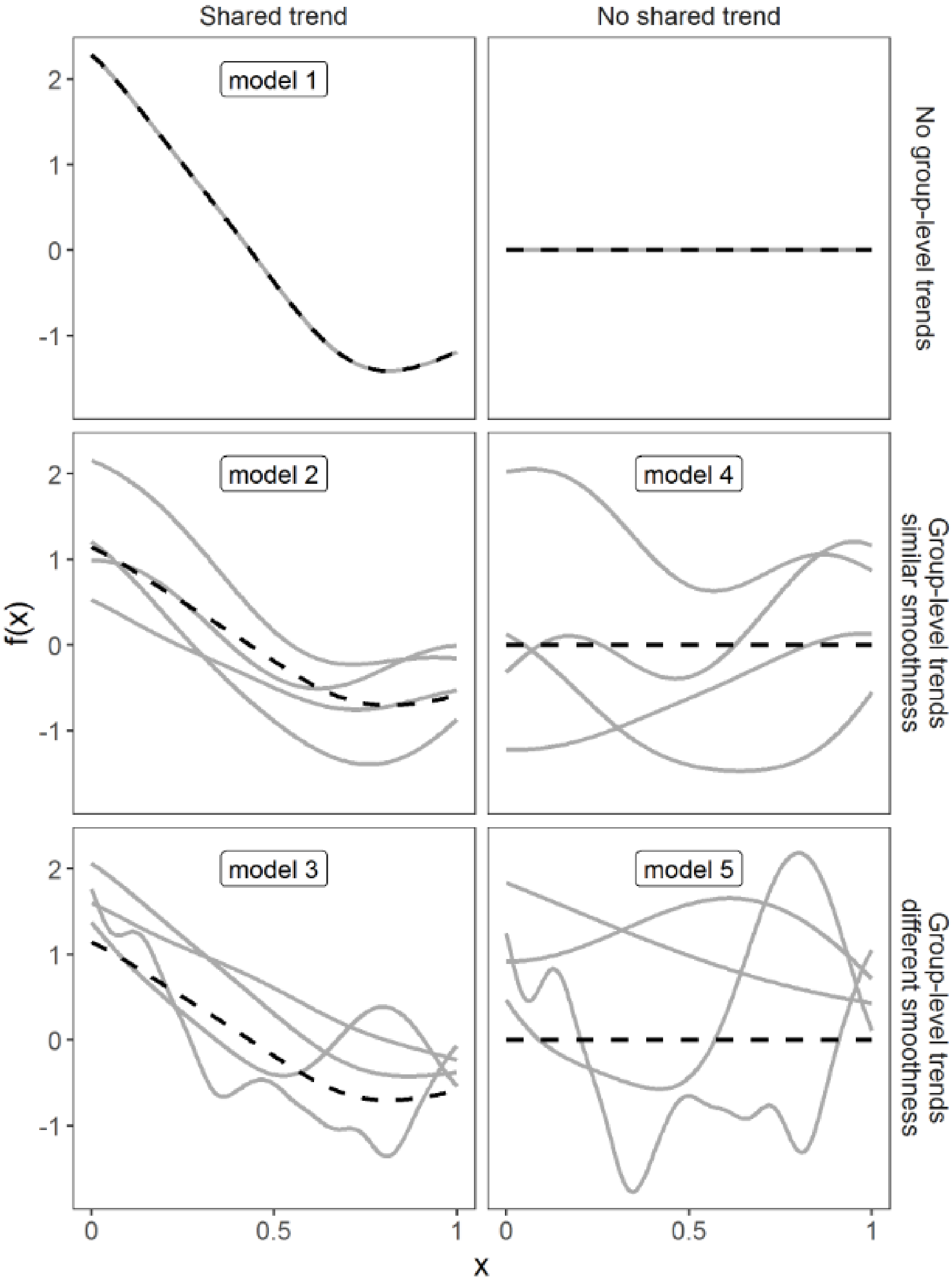
```
g3 <- gam(mpg ~ s(hp) + s(wt), data = mtcars)
draw(g3)
```




```r
concurvity(g3)
```

```
                 para     s(hp)     s(wt)
worst    2.534737e-18 0.9575001 0.9575001
observed 2.534737e-18 0.6883189 0.6968782
estimate 2.534737e-18 0.4784240 0.7978191
```

Many options: simple random effects (`bs = "re"`); *cyclic* splines (make $x(0) = x(T)$; `bs="cc"`) ; multidimensional splines (thin-plate, *tensor product* (`te()`); spherical (*Duchon*) splines (`bs = "sos"`); Markov random fields (`bs = "mrf"`); Gaussian processes (`bs = "gp"`); splines by category (`by=` argument); hierarchical splines (Pedersen et al. 2019); constrained splines (`scam` package, Pya and Wood (2015)); *soap film* splines; etc etc etc etc …


Shared trend
No shared trend
model 1
No group-level trends
model 2
model 4
Group-level trends similar smoothness
model 3
model 5
Group-level trends different smoothness
f(x)
x
2
1
0
-1
0
0.5
1

Duality between $\mathbf{Z}$ and correlation structure

- Hefley et al. (2017)
- "first-order specification": $\mathbf{y} \sim N(\mathbf{X}\beta + \mathbf{Z}\mathbf{b}, \sigma^2_\epsilon \mathbf{I})$
- "second-order specification: $\mathbf{y} \sim N(\mathbf{X}\beta, \sigma^2_\epsilon \mathbf{I} + \sigma^2_\mathbf{b}\Sigma)$
- if $\mathbf{b}$ are iid Normal, integrating first-order specification shows that $\Sigma = \mathbf{Z}\mathbf{Z}^\top$
- e.g. latent-variable specification of an AR1 correlation structure
- e.g. `phyloglmm`

Penalty matrices as

- Simon N. Wood (2004)

Computational tricks

- work with *precision matrix* where possible Σ^{-1}
- for a **multivariate normal** response, $\Sigma^{-1}_{ij} = \Sigma^{-1}_{ji} = 0 \leftrightarrow x_i$ and x_j are **conditionally independent**
- e.g. precision matrix of AR1 is tridiagonal with diagonal $1+\rho^2$, first off-diagonal elements $-\rho$ (see here)
- work with *reduced-rank* forms where necessary

Golub, Gene H., Michael Heath, and Grace Wahba. 1979. "Generalized Cross-Validation as a Method for Choosing a Good Ridge Parameter." *Technometrics* 21 (2): 215–23. https://doi.org/10.1080/00401706.1979.10489751.

Hastie, T. J., and R. J. Tibshirani. 1990. *Generalized Additive Models*. CRC Press.

Hastie, Trevor, Robert Tibshirani, and J. H Friedman. 2009. *The Elements of Statistical Learning: Data Mining, Inference, and Prediction*. New York: Springer. https://hastie.su.domains/Papers/ESLII.pdf.

Hefley, Trevor J., Kristin M. Broms, Brian M. Brost, Frances E. Buderman, Shannon L. Kay, Henry R. Scharf, John R. Tipton, Perry J. Williams, and Mevin B. Hooten. 2017. "The Basis Function Approach for Modeling Autocorrelation in Ecological Data." *Ecology* 98 (3): 632–46. https://doi.org/10.1002/ecy.1674.

Larsen, Kim. 2015. "GAM: The Predictive Modeling Silver Bullet | Stitch Fix Technology – Multithreaded." *MultiThreaded (StitchFix)*. https://multithreaded.stitchfix.com/blog/2015/07/30/gam/.

Pedersen, Eric J., David L. Miller, Gavin L. Simpson, and Noam Ross. 2019. "Hierarchical Generalized Additive Models in Ecology: An Introduction with Mgcv." *PeerJ* 7 (May): e6876. https://doi.org/10.7717/peerj.6876.

Perperoglou, Aris, Willi Sauerbrei, Michal Abrahamowicz, and Matthias Schmid. 2019. "A Review of Spline Function Procedures in R." *BMC Medical Research Methodology* 19 (1): 46. https://doi.org/10.1186/s12874-019-0666-3.

Pya, Natalya, and Simon N. Wood. 2015. "Shape Constrained Additive Models." *Statistics and Computing* 25 (3): 543–59. https://doi.org/10.1007/s11222-013-9448-7.

Ramsay, Timothy O., Richard T. Burnett, and Daniel Krewski. 2003. "The Effect of Concurvity in Generalized Additive Models Linking Mortality to Ambient Particulate Matter." *Epidemiology* 14 (1): 18. https://journals.lww.com/epidem/Fulltext/2003/01000/The_Effect_of_Concurvity_in_Generalized_Additive.9.aspx.

Wood, Simon N. 2004. "Stable and Efficient Multiple Smoothing Parameter Estimation for Generalized Additive Models." *Journal of the American Statistical Association* 99 (467): 673–86. https://doi.org/10.1198/016214504000000980.

Wood, Simon N. 2017. *Generalized Additive Models: An Introduction with R.* CRC Texts in Statistical Science. Chapman & Hall.