Splines and basis expansion (week 3?)

7 Feb 2023

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linear basis expansion

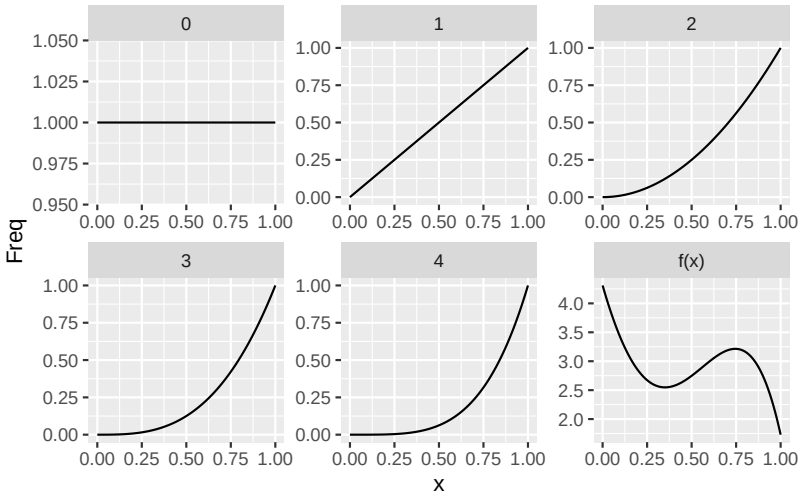
- transformations of various kinds
- quadratic expansion
- nonlinear transformations
- indicator variables

Select or regularize from the expanded set.

polynomial basis

- polynomial basis: $y_i = \sum_{j=0}^{n} \beta_j x_i^j$

```
## replicate figure 3.2 from Wood
library(ggplot2)
x <- seq(0, 1, length = 101)
n <- 4
y <- sapply(0:n, \(j) x^j)
beta <- c(4.31, -10.72, 16.8, 2.22, -10.88)
y <- cbind(y, fx = y %*% beta)
dimnames(y) <- list(x = x, j = c(0:n, "f(x)"))
yy <- as.data.frame(as.table(y))
yy$x <- as.numeric(as.character(yy$x))
ggplot(yy, aes(x, Freq)) + geom_line() + facet_wrap(~j, scale = "free")
```



piecewise polynomial bases

- constant, linear, continuous
- basis functions
- translate from x_i to columns of $\mathbf{X}$

splines

- **piecewise** polynomials with continuity/smoothness constraints
- very useful for function approximation
- convert a single numeric predictor into a flexible basis
- efficient
- with multiple predictors, consider **additive models**
- handle interactions (multidim smooth surfaces) *if reasonably low-dimensional*: tensor products etc.

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

truncated power basis

- $X^0 \ldots X^n$
- remaining columns are $(x - \xi_\ell)+^{M-1}$ where ℓ are the *interior knots*

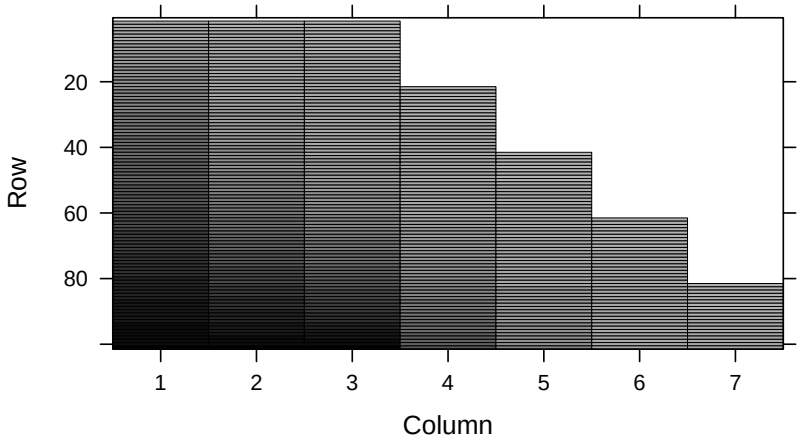
truncated power basis

- **Kronecker product**: blockwise multiplication ($\mathbf{A} \bigotimes \mathbf{B}$ multiplies $\mathbf{B}$ by each a_{ij})
- **Khatri-Rao product**: columnwise Kronecker product
  - super-handy for combining indicator variables with

```
truncpolyspline <- function(x, df) {
    if (!require("Matrix")) stop("need Matrix package")
    knots <- quantile(x, seq(0, 1, length = df - 1))
    ## should probably use seq() instead of `:`
    ## dim: n x (df-2)
    trunc_fun <- function(k) (x>=k)*(x-k)^3
    S <- sapply(knots[1:(df-2)], trunc_fun)
    S <- as(S, "CsparseMatrix")
    ## dim: n x df
    S <- cbind(x, x^2, S)
    return(S)
}
xvec <- seq(0, 1, length = 101)
tS <- truncpolyspline(xvec, df = 7)
```

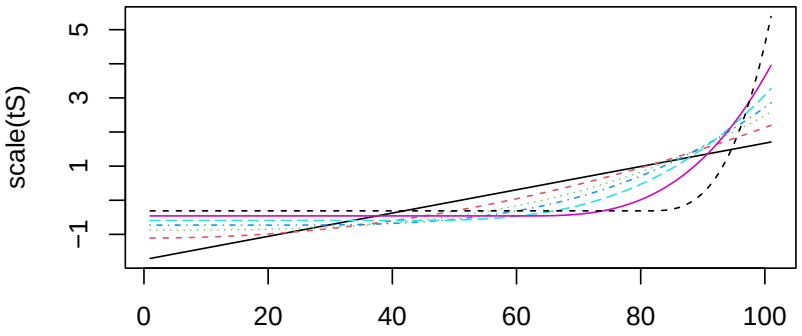
```
Loading required package: Matrix
```

```
image(tS, aspect = "fill")
```

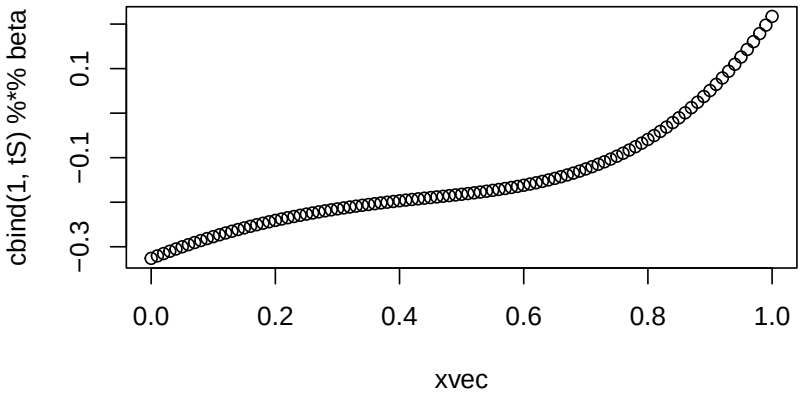


Dimensions: 101 x 7

```
matplot(scale(tS), type = "l")
```




```
set.seed(101)
beta <- rnorm(8)
plot(xvec, cbind(1, tS) %*% beta)
```



Alternatively: create directly in sparse format.

- `d`: numeric (double-precision), vs `l` (logical), `n` (position)
- `g`: general, vs. `t` (triangular), `s` (symmetric)
- `C`: compressed sparse column form, vs. `R` (row form); `T` (triplet form)

compressed sparse column form

- `@i`: vector of row-**i**ndices (0-indexed??)
- `@p`: (0-indexed) vector of **p**ointers to starting elements of each column
- `@x`: values

e.g. `M@i[M@p[4]+1]` is the row-index of the first non-zero element in the fourth column; `M@x[M@p[4]+1]` is the value of the first non-zero element in the fourth column

```
truncpolyspline2 <- function(x, df) {
    knots <- quantile(x, seq(0, 1, length = df - 1))
    nx <- length(x)
    iL <- list()
    pL <- list()
    xL <- list()
    n <- 3
    j <- 0
    pL[[1]] <- 0L
    for (i in 1:(n-1)) {
```

```
        j <- j+1
        xL[[j]] <- x^i
        iL[[j]] <- seq(nx)-1L
        pL[[j+1]] <- i*nx
    }
    for  (i in 1:(df-2)) {
        j <- j+1
        ## figure out number of non-zero elements
        ## (could squeeze out a bit more here by counting up)
        nzk <- sum(x < knots[i])
        pos <- (nzk+1):nx
        xL[[j]] <- (x[pos]-knots[i])^3
        iL[[j]] <- pos-1L
        pL[[j+1]] <- pL[[length(pL)]]+(nx-nzk)
    }
    new("dgCMatrix", i = unlist(iL), p = unlist(pL), x = unlist(xL),
        Dim = c(nx, as.integer(df)))
}
tS2 <- truncpolyspline2(xvec, df = 7)
all.equal(unname(tS), tS2) ## TRUE
```

```
[1] TRUE
```

```
identical(unname(matrix(tS)), matrix(tS2))  ## TRUE
```

```
[1] TRUE
```

B-spline basis

- splines of a given order with *minimal support* (i.e., local)
- basis functions defined by recursion (not pretty)
- convenient for regression splines (see below)

natural cubic splines

- linear constraints beyond boundary knots (so 2d and 3d derivatives are 0 at the boundaries)

```
library(splines)
bb <- bs(1:20, df = 5)
attributes(bb)[c("degree", "knots", "Boundary.knots")]
```

```
$degree
[1] 3

$knots
33.33333% 66.66667%
 7.333333 13.666667

$Boundary.knots
[1]  1 20
```

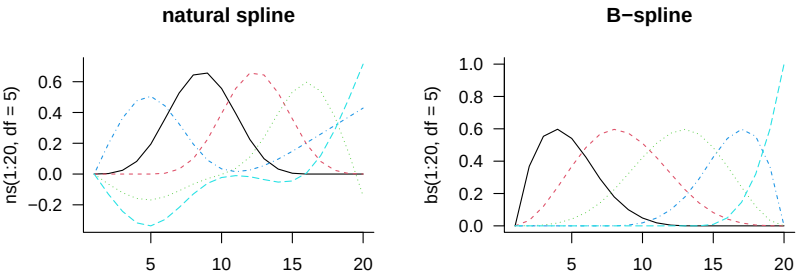
```
nn <- ns(1:20, df = 7)
attributes(nn)[c("degree", "knots", "Boundary.knots")]
```

```
$degree
[1] 3

$knots
14.28571% 28.57143% 42.85714% 57.14286% 71.42857% 85.71429%
 3.714286  6.428571  9.142857 11.857143 14.571429 17.285714

$Boundary.knots
[1]  1 20
```

```
par(mfrow = c(1,2),las =1, bty ="l")
matplot(ns(1:20, df = 5), type = "l", main = "natural spline")
matplot(bs(1:20, df = 5), type = "l", main = "B-spline")
```

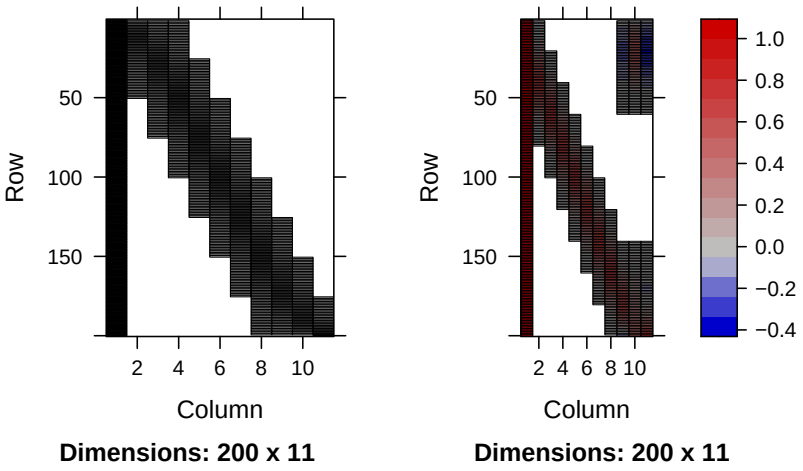


variance of predictions

- suppose $\mathbf{V}$ = variance of coefficient β
- then covariance matrix of predictions $\mathbf{X}\beta$ is $\mathbf{XVX}^\top$
- Variance of predictions, brute force: Diag($\mathbf{XVX}^\top$)
- Clever: compute diagonal directly
  - `emulator::quad.diag` (`colSums(crossprod(M, Conj(tx)) * tx)`)

sparsity patterns

```
library(Matrix)
dd <- data.frame(x=1:200)
Xb <- model.matrix(~splines::bs(x, df = 10), data = dd)
Xn <- model.matrix(~splines::ns(x, df = 10), data = dd)
gridExtra::grid.arrange(
               ncol = 2,
               image(Matrix(Xb), aspect = "fill"),
               image(Matrix(Xn), aspect = "fill")
               )
```



examples: South African heart disease

- use splines in a GLM with no additional effort
- fit splines to all continuous variables
- ESL says "use four natural spline bases" (… elements??)
- i.e. `df = 4` (no intercept)
- stepwise deletion via AIC
- why??
- showing p-values (why???)
- `stepAIC(..., direction = "backward")`

phoneme example

- combination of feature transformation (time to Fourier domain) and regularization
- smooth first, regress afterwards

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

$$(\mathbf{y} - \mathbf{N}\theta)^\top(\mathbf{y} - \mathbf{N}\theta) + \lambda\theta^\top\Omega_N\theta$$

with $\{\Omega_N\}_{jk} = \int N_j''(t)N_k''(t)\,dt$ $$ **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" of Ω_N

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

degrees of freedom and smoother matrix

- The equivalent of the hat matrix is

$$\mathbf{N}(\mathbf{N}^\top\mathbf{N} + \lambda\Omega_N)^{-1}\mathbf{N}^\top$$

- "Smoother matrix"
- hat matrix is *idempotent* (why?), smoother matrix is *shrinking*
- smoother matrix has lower rank
- effective degrees of freedom = trace of hat matrix (again)

reduced-rank splines

- We *can* use as many knots as observations, but do we really need to?
- From `?mgcv::s`:

> … exact choice of 'k' is not generally critical: it should be chosen to be large enough that you are reasonably sure of having enough degrees of freedom to represent the underlying `truth' reasonably well, but small enough to maintain reasonable computational efficiency. Clearly`large' and 'small' are dependent on the particular problem being addressed.

———. 2017. *Generalized Additive Models: An Introduction with R*. CRC Texts in Statistical Science. Chapman & Hall. https://www.amazon.com/Generalized-Additive-Models-Introduction-Statistical-ebook/dp/B071Z9L5D5/ref=sr_1_1?ie=UTF8&qid=1511887995&sr=8-1&keywords=wood+additive+models.

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.

The default basis dimension, 'k', is the larger of 10 and 'm[1]' (spline order)

fitting additive models (more than one): backfitting

Hastie and Tibshirani (1987)

Hastie, Trevor, and Robert Tibshirani. 1987. "Generalized Additive Models: Some Applications." *Journal of the American Statistical Association* 82 (398): 371–86. https://doi.org/10.1080/01621459.1987.10478440.

- scatterplot smoother ($S()$: **any** smoothing method, e.g. local linear or kernel estimation)
- **backfitting**
  - take partial residuals: $r_{ij} = y_i - \hat{\alpha} - \sum_{k \neq j} \hat{f}_k(X_{ki})$
  - smooth them ($\hat{f}_j(x_{ji}) = S(r_j | x_{ji})$)
- either do a *cyclic* fit (backfitting), fitting on partial residuals each time
- can do *semiparametric* fitting (some regular linear terms, some smoothed terms)
- **local scoring**

$$
\begin{aligned}
\hat{\eta} &= \hat{\alpha} + \sum \hat{f}_j \\
\hat{\mu} &= g^{-1}(\hat{\eta}) \\
\mathbf{z} &= \hat{\eta} + (y - \mu)/V(\mu) \\
\mathbf{w} &= \mathrm{Diag}(1/V(\mu))
\end{aligned}
$$

Now do back-fitting (instead of weighted least squares) on $\mathbf{z}$ with weights $\mathbf{w}$

historical note

- Backfitting was developed in the context of **alternating conditional expectations** (Breiman and Friedman 1985); finding optimal transformations for the response and each of the variables in a multivariate regression.
- Univariate ACE is like backfitting but alternating between transformations for y and x rather than among the different predictor variables
- `acepack` package for R

Breiman, Leo, and Jerome H. Friedman. 1985. "Estimating Optimal Transformations for Multiple Regression and Correlation." *Journal of the American Statistical Association* 80 (391): 580–98. https://doi.org/10.1080/01621459.1985.10478157.

fitting additive models: alternative

- stuff the whole thing into one giant GLM with appropriate penalization
-

generalized cross-validation

Larsen (2015), Golub, Heath, and Wahba (1979)

- minimize $\mathrm{RSS}/(\mathrm{Tr}(\mathbf{I} - \S(\lambda)))^2$
- "a rotation-invariant version of PRESS" $(\sum(e_i/(1 - h_i i))^2)$

REML criterion

- Reiss and Todd Ogden (2009), Wood (2011)
- less likely to overfit than GCV
- reduced tendency to multiple minima

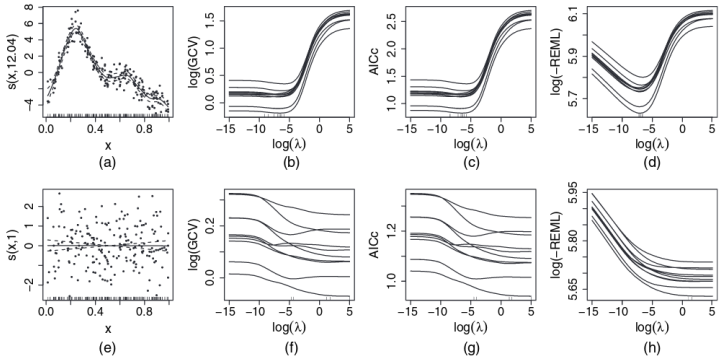


Fig. 1. Example comparison of GCV, AICc and REML criteria: (a) some (x,y)-data modelled as $y_i = f(x_i) + \varepsilon_i$, ε_i independent and identically distributed $N(0,\sigma^2)$ where smooth function f was represented by using a rank 20 thin plate regression spline (Wood, 2003); (b)–(d) various smoothness selection criteria plotted against logarithmic smoothing parameters, for 10 replicates of the data (each generated from the same 'truth') (note how shallow the GCV and AICc minima are relative to the sampling variability, resulting in rather variable optimal λ-values (which are shown as a rug plot), and a propensity to undersmooth; in contrast the REML optima are much better defined, relative to the sampling variability, resulting in a smaller range of λ-estimates); (e)–(h) are equivalent to (a)–(d), but for data with no signal, so that the appropriate smoothing parameter should tend to ∞ (note GCV's and AICc's occasional multiple minima and undersmoothing in this case, compared with the excellent behaviour of REML; ML (which is not shown) has a similar shape to REML)

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

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.

Reiss, Philip T., and R. Todd Ogden. 2009. "Smoothing Parameter Selection for a Class of Semiparametric Linear Models." *Journal of the Royal Statistical Society: Series B (Statistical Methodology)* 71 (2): 505–23. https://doi.org/10.1111/j.1467-9868.2008.00695.x.

Wood, Simon N. 2011. "Fast Stable Restricted Maximum Likelihood and Marginal Likelihood Estimation of Semiparametric Generalized Linear Models." *Journal of the Royal Statistical Society: Series B (Statistical Methodology)* 73 (1): 3–36. https://doi.org/10.1111/j.1467-9868.2010.00749.x.

computing the REML criterion

- Laplace approximation

multidimensional splines

tensor product

thin-plate splines

null space