# Moving Beyond Linearity

#### ACTL3142 & ACTL5110 Statistical Machine Learning for Risk Applications

Some of the figures in this presentation are taken from "An Introduction to Statistical Learning, with applications in R" (Springer, 2013) with permission from the authors: G. James, D. Witten, T. Hastie and R. Tibshirani



#### **Lecture Outline**

#### **Linearity & Nonlinearity**

- Data Science Starts With Data
- Linear Regression
- Polynomial Regression
- Step Functions
- Regression Splines
- Smoothing Splines
- Local Regression
- Generalised Additive Models (GAMs)



#### Nonlinear curves

The legend of the Laffer curve goes like this: Arthur Laffer, then an economics professor at the University of Chicago, had dinner one night in 1974 with Dick Cheney, Donald Rumsfeld, and *Wall Street Journal* editor Jude Wanniski at an upscale hotel restaurant in Washington DC. They were tussling over President Ford's tax plan, and eventually, as intellectuals do when the tussling gets heavy, Laffer commandeered a napkin and drew a picture. The picture looked like this: Laffer curve





#### One predictor vs multiple predictors

sales  $\approx \beta_0 + \beta_1 \times \texttt{TV}$ 







Multiple linear regression



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Source: James et al. (2021), *An Introduction to Statistical Learning with Applications in R*, Figures 3.1 & 3.5.

### By the end of today





Instead of just fitting lines (linear regression) or hyperplanes (multiple linear regression)…

You'll be able to fit nonlinear curves to multivariate data using *splines* and *Generalised Additive Models*.



Source: James et al. (2021), *An Introduction to Statistical Learning with Applications in R*, Figures 2.4 & 2.6.

## Moving beyond linearity

Using a term like nonlinear science is like referring to the bulk of zoology as the study of non-elephant animals. (Stanisław Ulam)

- Linear models are highly interpretable
- Linear assumption can be *very* unrealistic
- Look for interpretable nonlinear models
- A machine learning view, not a statistical view
- 1. Polynomial regression
- 2. Step functions
- 3. Regression splines
- 4. Smoothing splines
- 5. Local regression
- 6. Generalised additive models



#### In-class demonstration





Some mystery data

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#### **Instructions**

I want you to 'fit' the data four different ways by drawing:

**Top left**: a straight line

- Draw a single straight line
- Don't lift your pen from the page

**Bottom left**: a step function

- Draw a sequence of flat lines
- Lift your pen between each line

**Top right**: a quadratic curve

- Draw a single smiley-face curve
- Don't lift your pen from the page

**Bottom right**: a smooth curve

- Draw a single curve of any shape
- Avoid jagged changes of direction



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#### Luxembourg Mortality Data

Download a file called Mx\_1x1[.](https://www.mortality.org/) txt from the Human Mortality Database.

No-one is allowed to distribute the data, but you can download it for free. Here are the first few rows to get a sense of what it looks like.





#### Setup & importing the data

 $R$  Python

1 lux <- read\_table("Mx\_1x1.txt", skip = 2, show\_col\_types = FALSE) % 2 rename(age=Age, year=Year, mx=Female) %>% 3 select(age, year, mx) %>% 4 filter(age != '110+') %>% 5 mutate(year = as.integer(year), age = as.integer(age),  $mx = as.numeric(mx)$ )

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1 lux

# A tibble: 6,930 × 3

8 7 1960 0

10 9 1960 0 # ℹ 6,920 more rows

9 8 1960 0.000951

 age year mx <int> <int> <dbl> 1 0 1960 0.0239 2 1 1960 0.00169 3 2 1960 0.00171 4 3 1960 0.00126 5 4 1960 0.000844 6 5 1960 0.000873 7 6 1960 0.000443 1 summary(lux)



 $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$ 

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## Mortality

R Python



## Mortality (zoom in)

 $R \mid$  Python

1 lux  $\le$  lux  $\gg$  filter(age  $\le$  90)





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## Log-mortality

R Python

- 1 lux\$log\_mx <- log(lux\$mx)
- 2 lux <- lux[lux\$log\_mx != -Inf, ]





 $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$ 

#### Linear regression

 $R \mid Python$ 

- 1 lux\_2020 <- lux %>% filter(year == 2020 )
- 2 model\_lr <- lm(log\_mx ~ age, data = lux\_2020)





 $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$ 

#### Quadratic regression

 $R \mid Python$ 

1 model\_quad <-  $lm(log_mx \sim poly(age, 2)$ , data =  $lux_2020)$ 



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#### Step function regression

 $R \mid Python$ 

1 model\_step <-  $lm(log_mx \sim cut(age, seq(0, 90, 10), right=F), data = lux_2020)$ 



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## Regression spline

 $R \mid Python$ 

1 model\_spline <- lm(log\_mx  $\sim$  bs(age, degree=10), data=lux\_2020) # Requires splines package



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## Industry approaches



Methods from this class (p. 8–9):

- ridge regression
- lasso regression
- elastic net
- generalised linear models
- generalised additive models
- random forests
- dimension reduction
- (artificial neural networks)

Take **ACTL3141/ACTL5104** for mortality modelling, [IFoA bulletin on machine learning in](https://actuaries.org.uk/media/mwbojehy/longevity-bulletin-issue-15.pdf) **[ACTL3143/ACTL5111](https://laub.au/ai)** for actuarial AI [mortality modelling](https://actuaries.org.uk/media/mwbojehy/longevity-bulletin-issue-15.pdf)



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#### Plotting the fitted values

 $R$  Python

1 ggplot(lux\_2020, aes( $x = age$ ,  $y = log_mx$ )) + theme\_minimal() + 2 geom\_point(aes(y = predict(model\_lr)), color = "red", size = 2) + 3 geom\_point(alpha =  $0.75$ , size = 2) + labs(x = "Age", y = "Log-Mortality")





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## Linear regression with error bars

 $R$  Python

1 ggplot(lux\_2020, aes( $x = age$ ,  $y = log_mx$ )) + theme\_minimal() + 2 geom\_smooth(method = "lm", formula =  $y \sim x$ , color = "red", linewidth=2) + 3 geom\_point(alpha =  $0.75$ ) + labs(x = "Age", y = "Log Mortality")





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#### Interpolating

 $R \mid Python$ 

1 df\_grid <- data.frame(age = seq (25, 35, by = 0.5))

2 df\_grid \$log\_mx <- predict(model\_lr, newdata = df\_grid)





 $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$ 

#### Extrapolating

 $R \mid Python$ 

1 df\_grid <- data.frame(age = seq (40, 130))

2 df\_grid \$log\_mx <- predict(model\_lr, newdata = df\_grid)



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 $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$ 

#### Multiple linear regression

c ("age", "year", "log\_mx")]

2 head(df\_mlr)

# A tibble:  $6 \times 3$ 



- $\frac{1}{2} \frac{df_m \ln r}{head(df_m \ln r)}$ <br>  $\frac{4}{2} \frac{h \cdot 1}{h \cdot 1}$ <br>  $\frac{4}{2} \frac{h \cdot 1}{h \cdot 1}$ <br>  $\frac{4}{2} \frac{1}{2} \frac{1}{2}$ <br>  $\frac{1}{2} \frac{1}{2} \frac$  <int> <int> <dbl> 1 0 1960 -3.74 2 1 1960 -6.38
- 3 2 1960 -6.37 4 3 1960 -6.68
- 5 4 1960 -7.08 6 5 1960 -7.04

#### **Fitting**:

1 linear\_model <- lm(log\_mx ~ age + year, data = df\_mlr)

- 1 new\_point <- data.frame (year = 2040, age = 20 )
- 2 predict(linear\_model, newdata = new\_point)

#### $-8.66$

1 coef(linear\_model)

(Intercept) age year 34.58222358 0.07287039 -0.02191158



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#### Fitted multiple linear regression





#### Link to interactive notebook



See the [spline demo notebook](https://unsw-risk-and-actuarial-studies.github.io/ACTL3142/M6-Moving-Beyond-Linearity/splines.html) for a high-level view of these methods



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## Polynomial regression

Extend the standard linear model

$$
Y_i = \beta_0 + \beta_1 x_i + \varepsilon_i
$$

to

$$
Y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \cdots + \beta_d x_i^d + \varepsilon_i
$$

- Relaxes the assumption that predictor and response are linearly related
- Works almost identically to multiple linear regression, except the other "predictors" are just transformations of the initial predictor



### Quadratic regression (by hand)

 $df_pr \leftarrow data.f$ rame(age = lux\_2020\$age, age2 = lux\_2020\$age^2, log\_mx = lux\_2020\$log\_mx) 2 head(df\_pr)



We just tricked R into thinking that age2 is a separate variable!

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This is a linear model of a nonlinearly transformed variable.



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## The poly function

1 df\_pr <- data.frame(age =  $lux_2020$ \$age,  $log_mx = lux_2020$ \$ $log_mx)$ 2 head(df\_pr)

 age log\_mx  $0 -5.363176$  $6 - 8.111728$ 3 15 -6.949619 4 16 -8.040959 5 18 -7.389022 6 21 -8.159519

> $poly_model \leftarrow lm(log_mx \sim poly(age, 2),$  $\lceil$ <sup>o</sup> $\rceil$  $2$  data =  $df_pr$ ) 3 coef(poly\_model)

```
 (Intercept) poly(age, 2)1 poly(age, 2)2 
  -5.787494 14.534731 6.376355
```
Now we *can't* put in age^2 as a separate variable.

 $\binom{1}{1}$ 1 new\_input  $\le -$  data.frame(age = 20) 2 predict(poly\_model, newdata = new\_input)





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## Quadratic regression with error bars

- 1 ggplot(lux\_2020, aes(x = age, y = log\_mx)) + theme\_minimal() +
- 2  $\,$  stat\_smooth(method =  $\,$  "lm", formula = y  $\sim$  poly(x, 2), color = "red", linewidth=2) +
- 3  $\,$  geom\_point(alpha = 0.75) + labs(x =  $\,$ "Age", y =  $\,$ "Log–Mortality")  $\,$







#### Polynomial expansion

1 head(lux\$age)

[1] 0 1 2 3 4 5





```
1 age_poly <- model.matrix(\sim poly(age, 2, raw=TRUE), data = lux)
2 head(age_poly)
```

```
(Intercept) poly(age, 2, raw = TRUE)1 poly(age, 2, raw = TRUE)2<br>
1 0<br>
2<br>
1<br>
1<br>
2<br>
4
1 0 0 0
2 \qquad \qquad 1 \qquad \qquad 1 \qquad \qquad 13 \hspace{1.5cm} 1 \hspace{1.5cm} 2 \hspace{1.5cm} 44 1 3 9
5 1 4 16
\begin{array}{ccccccc} 6 & 1 & 5 & 25 \end{array}
```
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#### Monomials plotted (raw=TRUE)

 $1$  age\_poly <– model.matrix( $\sim$  poly(age,  $2$ , raw=TRUE), data = lux)





#### Orthogonal polynomials plotted (default)

age\_poly <- model.matrix( $\sim$  poly(age, 4), data = lux)



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## Why? Raw polynomials can be highly correlated

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Reciprocal of the condition number is rcond.

```
1 \text{ X} \leftarrow \text{model.matrix}(\sim \text{poly}(\text{age}, 10))data = lux)3 rcond(t(X) \frac{8}{5} x)
```
 $X$ <sub>raw <- model.matrix( $\sim$  poly(age, 10, raw= $E$ U</sub>  $2$  data = lux) 3  $rcond(t(X \text{ raw}) \text{ % } X \text{ raw})$ 

[1] 0.0002087683

[1] 1.155411e-40

We want it to be close to 1, so that the matrix can be inverted.

 $inv \leq -solve(t(X) \iff X)$  1 inv  $\leq -solve(t(X-ray) \iff X_{raw})$ 

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Error in solve.default(t(X\_raw) %\*% X\_raw): system is computationally singular: reciprocal condition  $number = 1.15541e-40$ 


### Example: Polynomial regression





## Can easily use polynomials in classification

Degree-4 Polynomial



(Right Side:) Model of binary event Wage > 250 via logistic regression

$$
\mathbb{P}(y_i > 250 | x_i) = \frac{\exp(\beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \beta_3 x_i^3 + \beta_4 x_i^4)}{1 + \exp(\beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \beta_3 x_i^3 + \beta_4 x_i^4)}
$$

Source: James et al. (2021), *An Introduction to Statistical Learning with Applications in R*, Figure 7.1.

#### Polynomial regression: notes and problems Pros:

- Can model more complex relationships
- Can also use this in logistic regression, or any linear-like regression for that matter

Cons:

- Normally stick to polynomials of degree 2-4; shape can get very erratic with higher degrees
- Can be computationally unstable with high degrees
- Can be difficult to interpret
- Non-local effects in the errors



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# Step functions

Polynomial regression imposes a *global structure* on the nonlinear function; an alternative is to use step functions.

Break up range of x into k distinct regions

$$
c_0
$$

Do a least squares fit on

 $y_i = \beta_0 + \beta_1 I(c_1 \leq x_i \leq c_2) + \beta_2 I(c_2 \leq x_i < c_3) + \cdots + \beta_{k-1} I(c_{k-1} \leq x_i \leq c_k)$ 

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## Example: Step functions



#### Step function regression on Wage data

**Piecewise Constant** 



Same Wage example as before but with step functions.

Source: James et al. (2021), *An Introduction to Statistical Learning with Applications in R*, Figure 7.2.



# Using I and cut





#### More general viewpoint: Basis functions Fit the model:

$$
y_i=\beta_0+\beta_1 b_1(x_i)+\beta_2 b_2(x_i)+\cdots+\beta_k b_k(x_i)
$$

- $b_1(x_i), b_2(x_i), \ldots, b_k(x_i)$  are the basis functions
- Transform the predictor before fitting it, and split it into multiple derived "predictors"

$$
\boldsymbol{X} = \begin{bmatrix} 1 & x_{11} & x_{12} & \ldots & x_{1p} \\ 1 & x_{21} & x_{22} & \ldots & x_{2p} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & \ldots & x_{np} \end{bmatrix} \qquad \boldsymbol{X} = \begin{bmatrix} 1 & b_1(x_1) & b_2(x_1) & \ldots & b_k(x_1) \\ 1 & b_1(x_2) & b_2(x_2) & \ldots & b_k(x_2) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & b_1(x_n) & b_2(x_n) & \ldots & b_k(x_n) \end{bmatrix}
$$

- For polynomial regression,  $b_j(x_i) = x_i^j$
- For step function regression,  $b_j(x_i) = I(c_j \leq x_i < c_{j+1})$  if  $j = 1, \ldots, k-1$



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### Example: Piecewise cubic regression

Example: Fitting a piecewise cubic polynomial with one "knot"

$$
y_i = \begin{cases}\beta_{0,1} + \beta_{1,1}x_i + \beta_{2,1}x_i^2 + \beta_{3,1}x_i^3 & \text{ if } x_i < c \\ \beta_{0,2} + \beta_{1,2}x_i + \beta_{2,2}x_i^2 + \beta_{3,2}x_i^3 & \text{ if } x_i \geq c\end{cases}
$$

is a knot: a point of our choosing where the model changes from one to another *c*

## Unconstrained cubic regression



Age

Unconstrained cubic regression on Wage data



# Spline definition

A piecewise polynomial function of degree d is a **spline** if the function is continuous up to the  $(d-1)$ th derivative at each knot.

- A 1st degree spline is a piecewise linear function which is continuous (i.e. the 0th derivative)
- A 2nd degree spline is a piecewise quadratic function which is continuous and has a continuous derivative
- A 3rd degree spline is a piecewise cubic function which is continuous and has continuous 1st and 2nd derivatives



#### Example: Linear spline

1 model <-  $lm(log_mx \sim bs(age, degree=1, knots=...), data = lux_2020)$ 





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#### Example: Cubic spline

1 model  $\leq$  lm(log\_mx  $\sim$  bs(age, degree=3, knots=...), data = lux\_2020)





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Four varieties of splines fit on a subset of the Wage data

Source: James et al. (2021), *An Introduction to Statistical Learning with Applications in R*, Figure 7.3.



# Cubic splines & natural splines

The cubic is preferred as it is the smallest order where the knots are not visible without close inspection.

We can extend the idea of a cubic spline to a **natural** cubic spline. It is a spline where outside the boundary knots (extrapolation) the function is linear.



Cubic spline & natural cubic spline fit to Wage subset Degree-15 spline & natural cubic spline fit to Wage data



Source: James et al. (2021), *An Introduction to Statistical Learning with Applications in R*, Figures 7.4 and 7.7.

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# Smoothing splines

Find a function g which minimises

$$
\frac{1}{n}\sum_{i=1}^n(y_i-g(x_i))^2+\lambda\int_{x=-\infty}^\infty g''(x)^2\,\mathrm{d}x
$$

- Goal: fit a function which minimises the MSE whilst still being 'smooth'
- *λ* is the tuning parameter which penalises a rougher fit
- $\lambda = 0$ : *g* will be very lumpy and will just interpolate all training data points (more flexible: less bias for more variance)
- $\lambda \to \infty$ : *g* will be a straight line fit (less flexible: more bias for less variance)
- turns out to be a (shrunken) natural cubic spline, with knots at every *g* training data point.

**Note**

For mortality smoothing, US uses smoothing splines, UK uses regression splines.



### Example: Smoothing splines

1 model <- smooth.spline(lux\_2020\$age, lux\_2020\$log\_mx, df = df)





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# Choosing *λ*

- : Effective degrees of freedom: measures the flexibility of the smoothing *df<sup>λ</sup>* spline.
	- Can be non-integer since some variables are constrained, so they are not free to vary
	- Note that the location and degree of the knots is all determined.
- Choice of  $\lambda$  via Cross validation.
- LOOCV error can be computed using only *one* computation for each  $\lambda$ ; extremely computationally efficient.



# Smoothing splines on Wage data

**Smoothing Spline** 





Comparing smoothing splines

Source: James et al. (2021), *An Introduction to Statistical Learning with Applications in R*, Figure 7.8.

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# Local regression

#### Algorithm

- 1. Get the fraction  $s = k/n$  nearest neighbours to the point  $x_0$
- 2. Assign each a weight  $K_{i0} = K(x_i, x_0)$  based on how close they are to  $x_0.$ Closer: higher weight. Furthest point in the *k* should get weight zero. Points outside the  $k$  selected should have a zero weight as well

3. Minimise

$$
\sum_{i=1}^n K_{i0}(y_i-\beta_0-\beta_1 x_i)^2
$$

$$
4. \ \hat{f}(x_0)=\hat{\beta}_0+\hat{\beta}_1x_0
$$



### Local regression example



Example of making predictions with local regression at  $x \approx 0.05$  and  $x \approx 0.45$ 

Source: James et al. (2021), *An Introduction to Statistical Learning with Applications in R*, Figure 7.9.

## Local regression cont.

- Local regression does a weighted regression of the points about some predictor value  $x_0.$  Can obtain an estimate for the response value at  $x_0$  from this
- Needs to be re-run each time an estimate at a different point is desired
- Useful for adapting model to recent data
- Possible to extend to 2 or 3 predictors: just have the weights based on distance in 2D or 3D space.
- Things start to get problematic if  $p > 4$  as there will be very few training observations



#### Local regression on Wage data

**Local Linear Regression** 



You can adjust the smoothness by changing the span

Source: James et al. (2021), *An Introduction to Statistical Learning with Applications in R*, Figure 7.10.



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#### GAMs

#### $y_i = \beta_0 + f_1(x_{i,1}) + f_2(x_{i,2}) + ... + f_p(x_{i,p}) + \varepsilon_i$

- Non-linearly fit multiple predictors on a response, whilst keeping the additive quality
- $f_i$  can be virtually  $\emph{any}$  function of the parameter, including the ones discussed earlier
- Find a separate  $f_i$  for each predictor, and add them together
- Can also be used on categorical responses in a logistic regression setting



## Example: GAM on Wage data



GAM fit using regression splines

- Each plot shows the contribution of each predictor to wage
- education is qualitative. The others are fit with natural cubic splines



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## Example: GAM on Wage data



GAM fit using smoothing splines

- Each plot shows the contribution of each predictor to wage
- education is qualitative. The others are fit with smoothing splines



# GAMs: pros and cons

- GAMs allow us to consider nonlinear relationships between the predictors and response, which can give a better fit
- Model is additive: can still interpret the effect of a single given predictor on the response
- However, model additivity ignores interaction effects between predictors. Could always add two-dimensional function parameters, e.g.  $f_{j,k}(x_j, x_k)$



# GAMs on Luxembourg data (mgcv)

 $model\_gam \leq gam(log\_mx \sim s(age) + s(year)$ , data=lux)

plot(model\_gam, select=1) 1 plot(model\_gam, select=2)





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#### GAMs on Luxembourg data (gam)

1 library(gam)

- 2 lux\_factor <- lux  $\gg$  mutate(year = factor(ye
- $3$  model\_gam <- gam(log\_mx  $\sim$  s(age) + year, data
- 4 plot(model gam)



1968 1972 1976 1980 1984 1988 1993 1997 2002 2007 2012 2017 2022









# **Glossary**

- interpolation & extrapolation
- polynomial regression
	- **monomials**
	- orthogonal polynomials
- step functions
	- basis function expansion
	- piecewise polynomial functions
- regression splines
	- **Exercise**
	- natural splines
	- cubic splines
- smoothing splines
- local regression
- generalised additive models (GAMs)



## Recommended viewing (splines)



[The Continuity of Splines](https://www.youtube.com/watch?v=jvPPXbo87ds)

It won't help with your assessment, it's just very entertaining/interesting.


# Recommended viewing (LOESS)

# **When Polynomials.** Don't Cut It



### R Package versions

1 print(sessionInfo(), locale=FALSE, tzone=FALSE)

R version 4.4.0 (2024-04-24) Platform: aarch64-apple-darwin20 Running under: macOS Sonoma 14.5

Matrix products: default BLAS: /Library/Frameworks/R.framework/Versions/4.4-arm64/Resources/lib/libRblas.0.dylib LAPACK: /Library/Frameworks/R.framework/Versions/4.4-arm64/Resources/lib/libRlapack.dylib; LAPACK version 3.12.0

attached base packages:

[1] splines stats graphics grDevices utils datasets methods [8] base

other attached packages:



loaded via a namespace (and not attached):



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# Python Package versions

1 from watermark import watermark

2 **print**(watermark(python=True, packages="matplotlib,numpy,pandas,seaborn,scipy"))

Python implementation: CPython Python version : 3.11.9<br>IPython version : 8.26.0 IPython version matplotlib: 3.9.0

numpy : 1.26.4 pandas : 2.2.2 seaborn : 0.13.2<br>scipy : 1.11.0 scipy



