A Journey through Functional Data and Dimension Reduction

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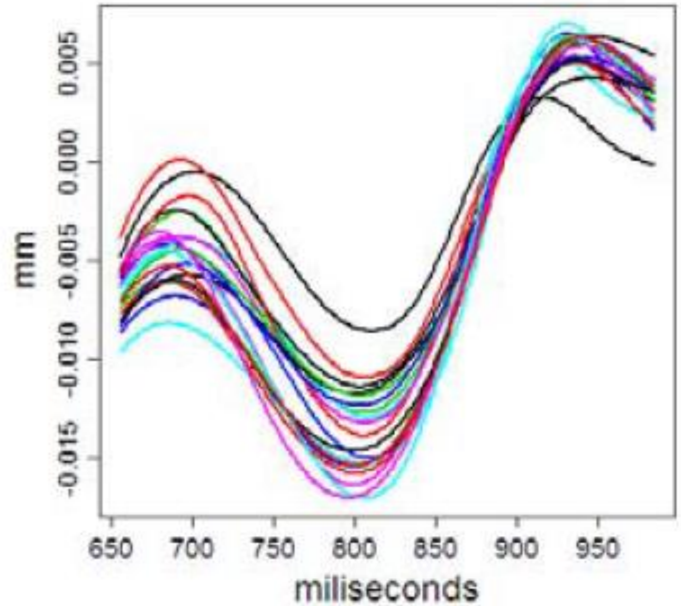
What is Functional Data?

20 replications



Functional data analysis involves repeated measures of the same process.

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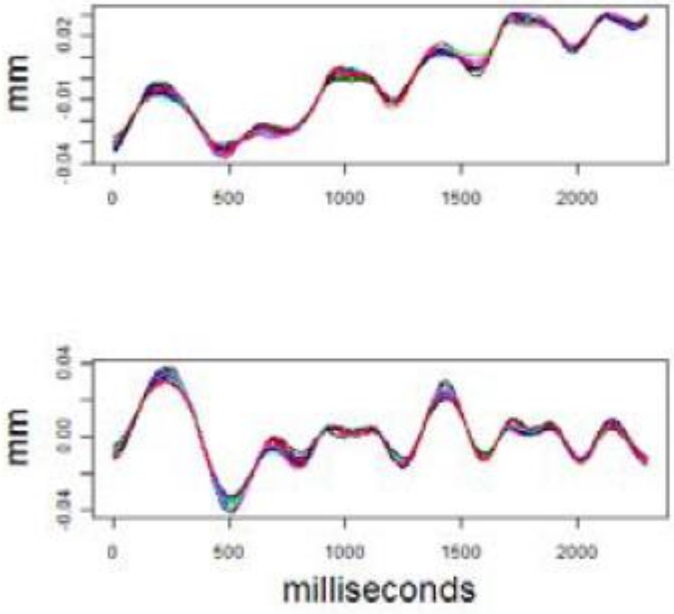
What is Functional Data?

20 replications, 1401 observations within replications, 2 dimensions



Functional data is often *complex*:

- often a large number of related quantities
- viewing each replication as a *single observation* can make the data easier to think about (once we have the right machinery)

- What are these data, anyway?

Some References

Three references for this course

- Ramsay & Silverman, 2005, "Functional Data Analysis"
- Ramsay & Silverman, 2002, "Applied Functional Data Analysis"
- Ramsay, Hooker & Graves, 2009, "Functional Data Analysis in R and Matlab"

- https://mehdi-m.shinyapps.io/fda-fpca/ (SHINY APP – IMPLEMENTED USING R)
- http://faculty.bscb.cornell.edu/~hooker/ShortCourseHandout.pdf (MAINLY USED THIS ONE TO PREPARE THE CURRENT SLIDE)

- https://www.stat.tamu.edu/~jianhua/paper/EJS-2008-218.pdf (Functional PCA)
- https://www.math.ntnu.no/emner/TMA4215/2008h/cubicsplines.pdf (Some Theory)
- http://www.cs.cmu.edu/~aarti/Class/10701_Spring14/ (ICA)
- http://faculty.washington.edu/dbp/s530/ (Wavelets)

Characteristics

- Data are measurements of smooth processes over time
- We usually do not want to make parametric assumptions about those processes.
- Often have multiple measurements of the same process
- We are interested in describing the variation of *processes*.
- Frequently, collected data have high resolution and low noise.
- Two (conflicting) goals: “fidelity” to y and “smoothness”
  - Fidelity, sum of squares: $\sum_{i=1}^{n} (y_i - x(t_i))^2$
  - How to quantify smoothness?

What Is Functional Data?

Functional data is multivariate data with an ordering on the dimensions. (Müller, (2006))

Key assumption is *smoothness*:

$$y_{ij} = x_i(t_{ij}) + \epsilon_{ij}$$

with t in a continuum (usually time), and $x_i(t)$ smooth

Functional data = the functions $x_i(t)$.

medical monitoring: EEG, ECG, fMRI, blood pressure ...

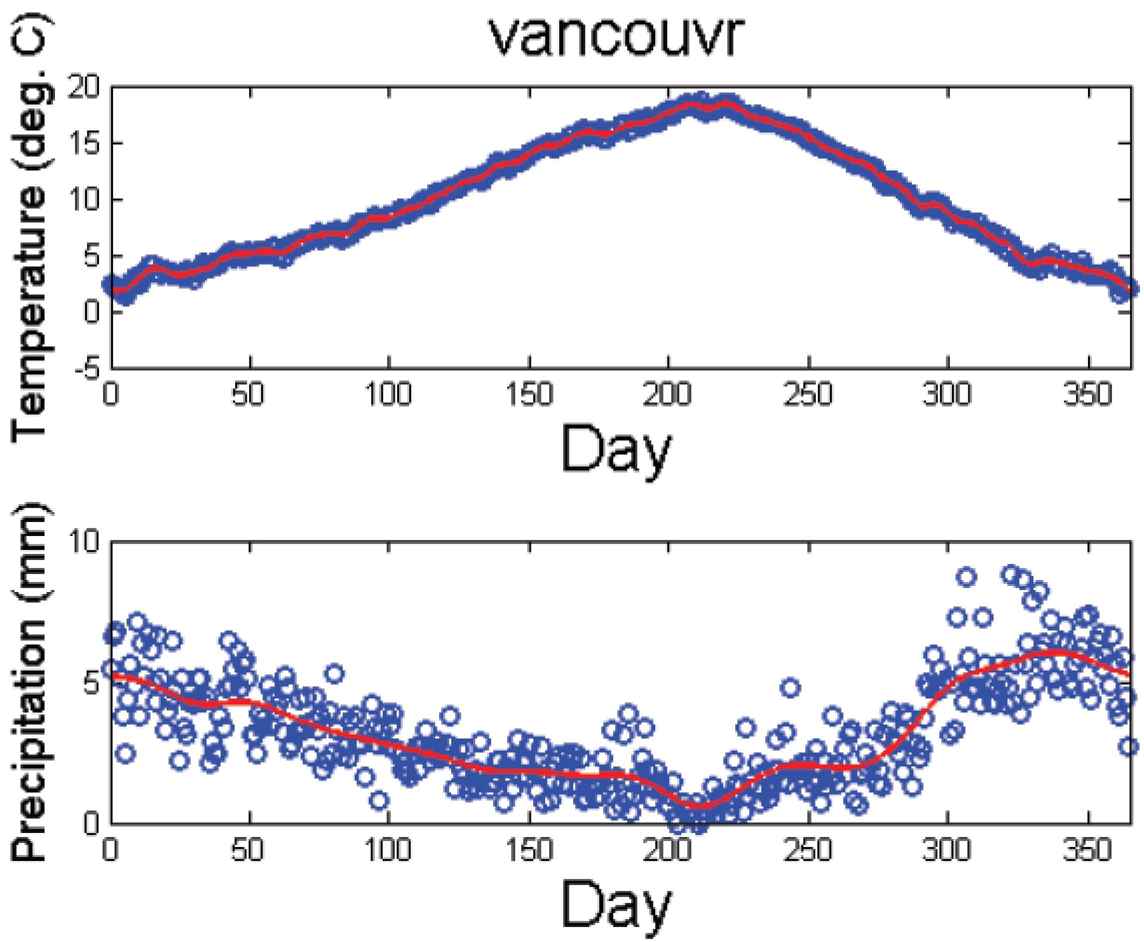
medical tests: HIV antibodies, flu screens...

biology: animal behavior (whale songs, fly egg-laying...)

environmental monitoring: weather, pollution, solar radiation, traffic ...

Weather In Vancouver

Measure of climate: daily precipitation and temperature in Vancouver, BC averaged over 40 years.



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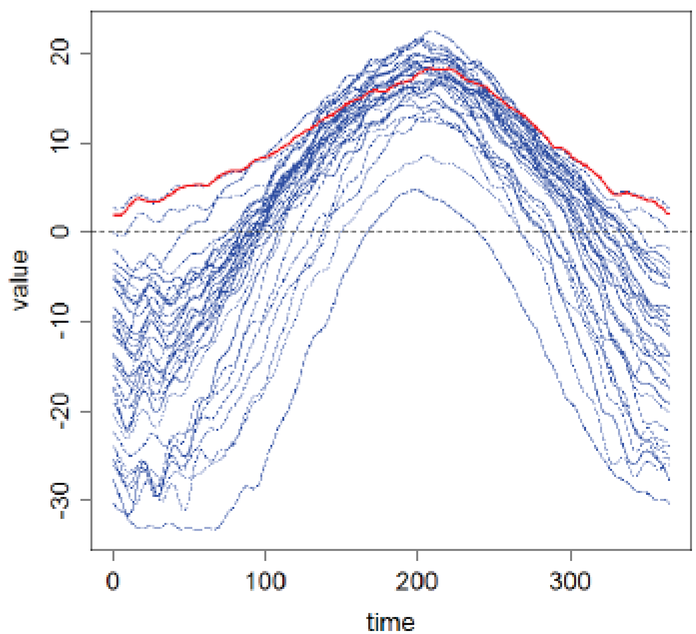
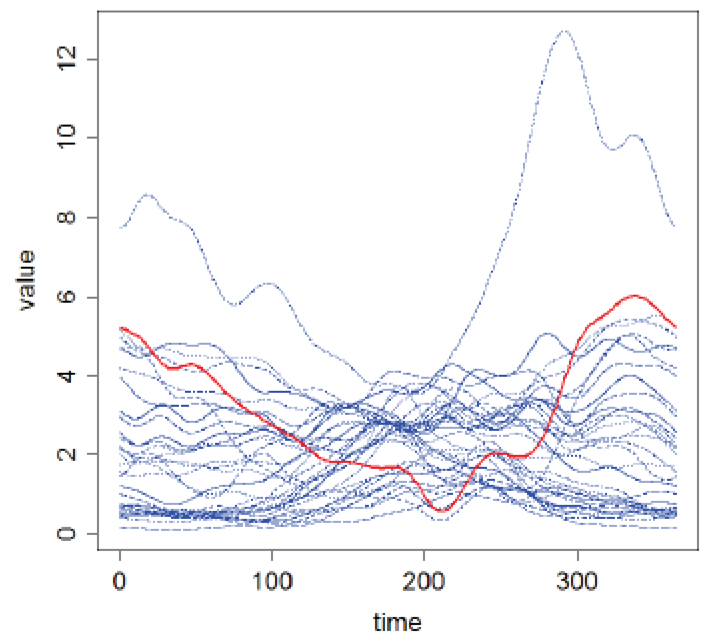
Canadian Weather Data

Average daily temperature and precipitation records in 35 weather stations across Canada (classical and much over-used)

Temperature



Precipitation



Interest is in variation in and relationships between smooth, underlying processes.

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What Are The Challenges?

- Estimation of functional data from noisy, discrete observations.
- Numerical representation of infinite-dimensional objects
- Representation of variation in infinite dimensions.
- Description of statistical relationships between infinite dimensional objects.
- $n < p = \infty$, and use of smoothness.
- Measures of variation in estimates.

Representing Functional Data

From Discrete to Functional Data

Two problems/two methods

1. Representing non-parametric continuous-time functions.
   - Basis-expansion methods:

$$x(t) = \sum_{i=1}^{K} \phi_i(t) c_i$$

     for pre-defined $\phi_i(t)$ and coefficients c_i.

2. Reducing noise in measurements
   - Smoothing penalties:

$$c = \operatorname{argmin} \sum_{i=1}^{n} (y_i - x(t_i))^2 + \lambda \int [Lx(t)]^2 \, dt$$

   - $Lx(t)$ measures "roughness" of x
   - λ a "smoothing parameter" that trades-off fit to the y_i and roughness; must be chosen.

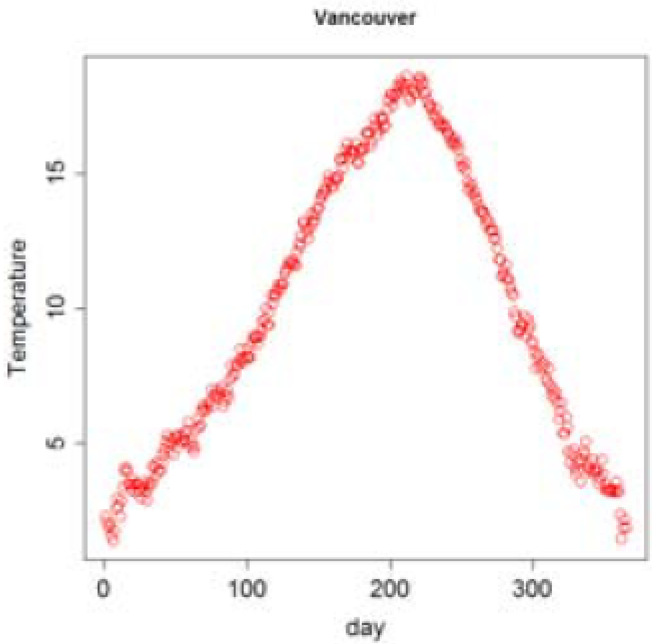
1. Basis Expansions

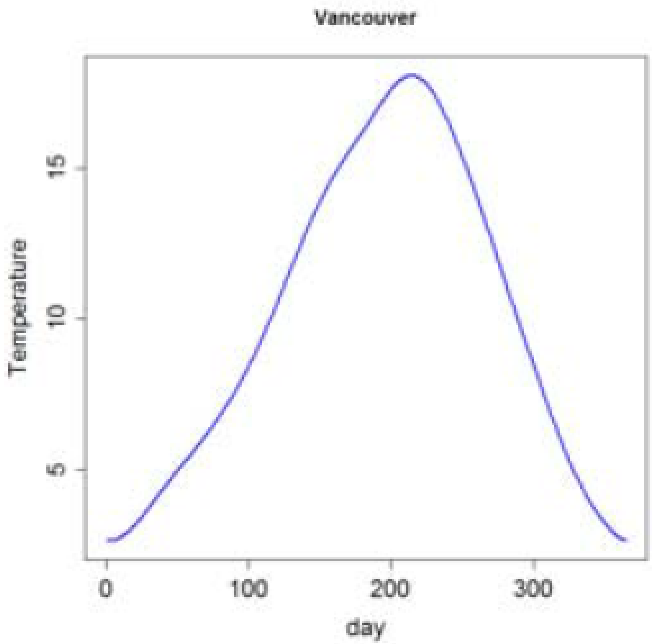
Univariate Case

From Data To Functions

How do we go from

data to functions?





Basis Expansions

From multiple linear regression:

$$y_i = \beta_0 + x_{1i}\beta_1 + x_{2i}\beta_2 + \cdots + \epsilon_i$$

Or if there is curvature:

$$y_i = \beta_0 + \beta_1 t_i + \beta_2 t_i^2 + \beta_3 t_i^3 + \cdots + \epsilon_i$$

Consider only one record

$$y_i = x(t_i) + \epsilon_i$$

represent $x(t)$ as

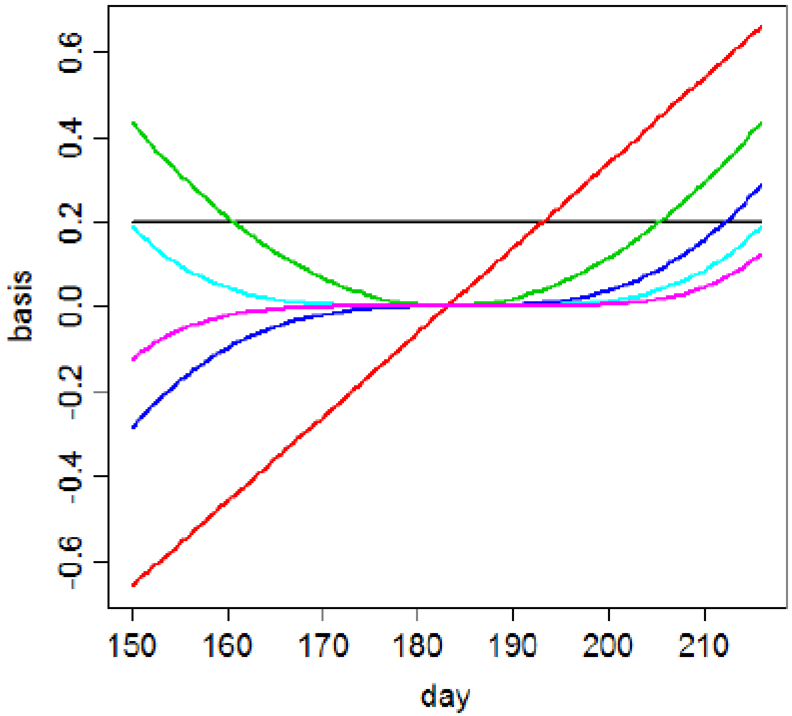
$$x(t) = \sum_{j=1}^{K} c_j \phi_j(t) = \Phi(t)\mathbf{c}$$

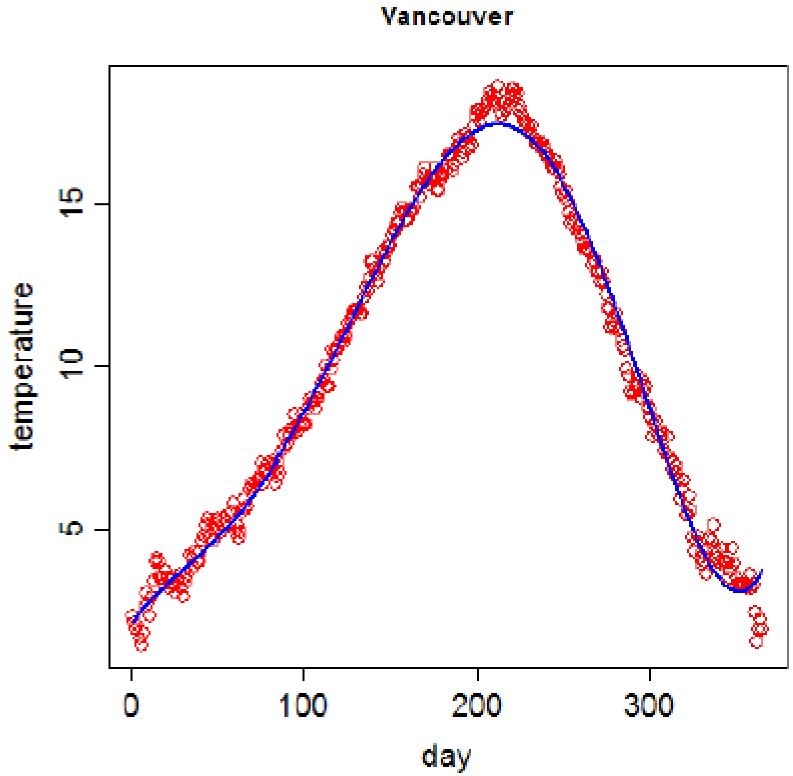
We say $\Phi(t)$ is a *basis system* for x.

$$x(t) = \beta_0 + \beta_1 t + \beta_2 t^2 + \beta_3 t^3 + \cdots$$

The Monomial Basis

$$\Phi(t) = (1, t, t^2, t^3, t^4, t^5, \ldots)$$





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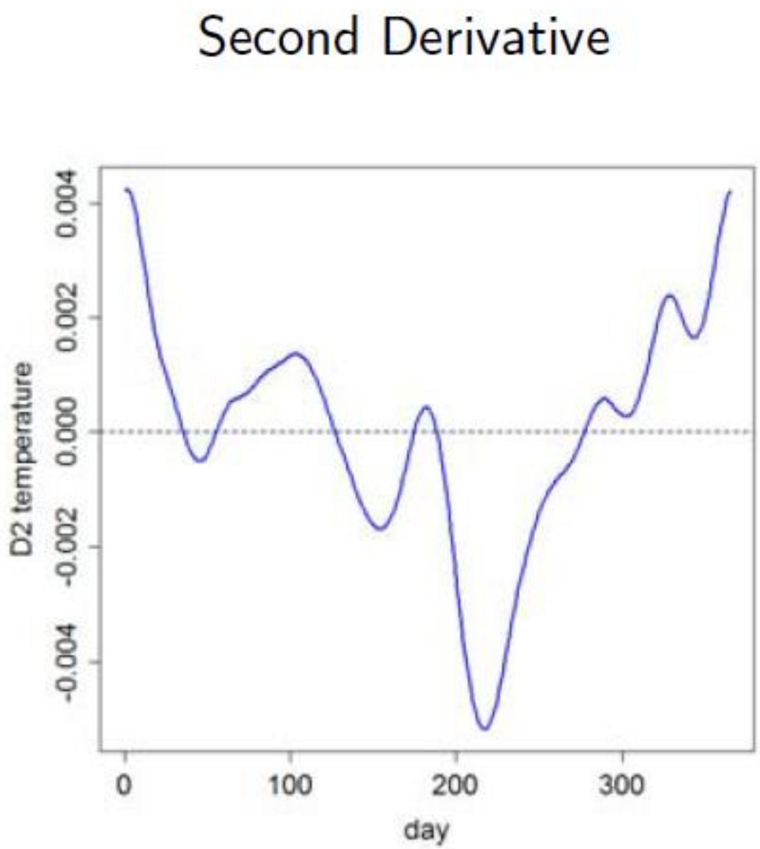
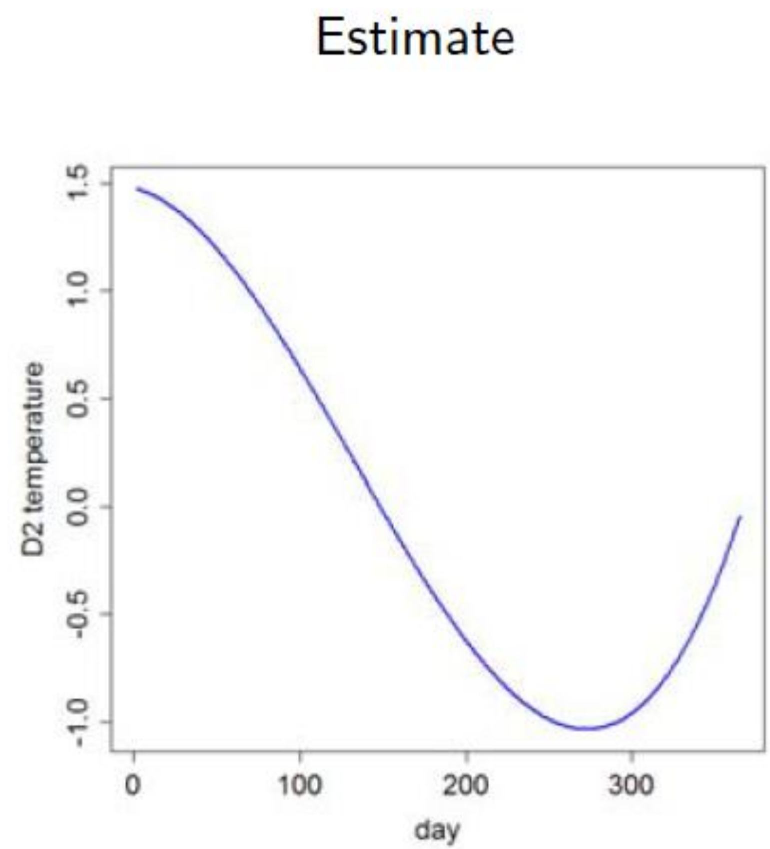
Problems with the Monomial Basis

Whereas the opposite happens in most real-world data:





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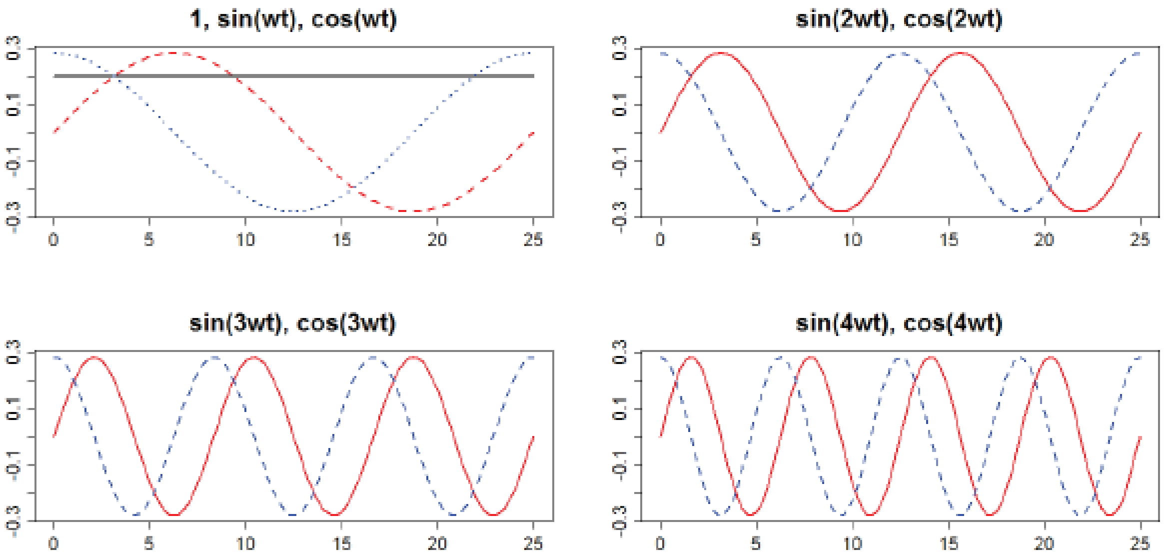
The Fourier Basis

- basis functions are sine and cosine functions of increasing frequency:

$$1, sin(\omega t), cos(\omega t), sin(2\omega t), cos(2\omega t), \ldots$$
$$sin(m\omega t), cos(m\omega t), \ldots$$

- constant $\omega = 2\pi/P$ defines the period P of oscillation of the first sine/cosine pair.



Advantages of Fourier Bases

- Only alternative to polynomials until the middle of the 20th century
- Excellent computational properties, especially if the observations are equally spaced.
- Natural for describing periodic data, such as the annual weather cycle

BUT representations are periodic; this can be a problem if the data are not.

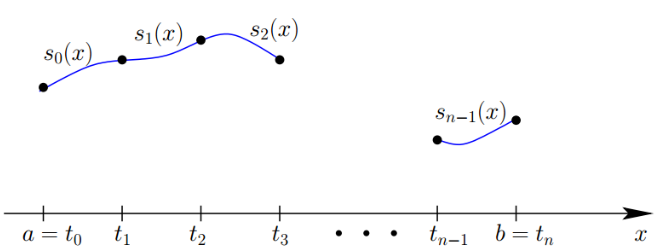
Fourier basis is first choice in many fields, eg signal processing.

Splines

- Splines are polynomial segments joined end-to-end
- Segments are constrained to be smooth at the join
- The points at which the segments join are called *knots*
- The order m (order = degree+1) of the polynomial segments and
- the location of the knots define the system.

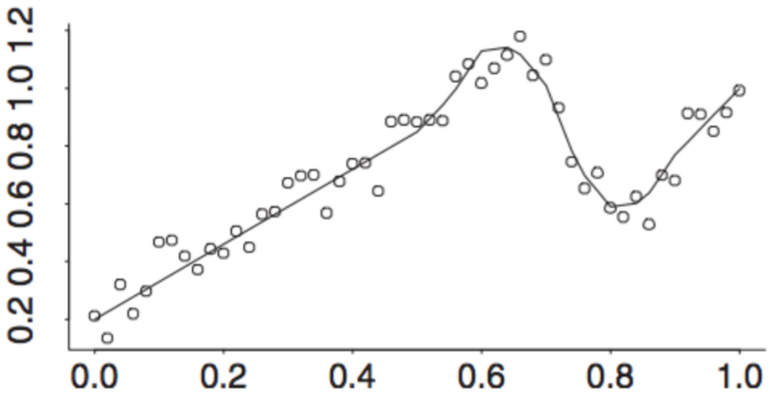
A function $S(x)$ is a spline of degree k on $[a, b]$ if

- $S \in C^{k-1}[a, b]$.
- $a = t_0 < t_1 < \cdots < t_n = b$ and



$$S(x) = \begin{cases} S_0(x), & t_0 \leq x \leq t_1 \\ S_1(x), & t_1 \leq x \leq t_2 \\ \vdots & \\ S_{n-1}(x), & t_{n-1} \leq x \leq t_n \end{cases}$$

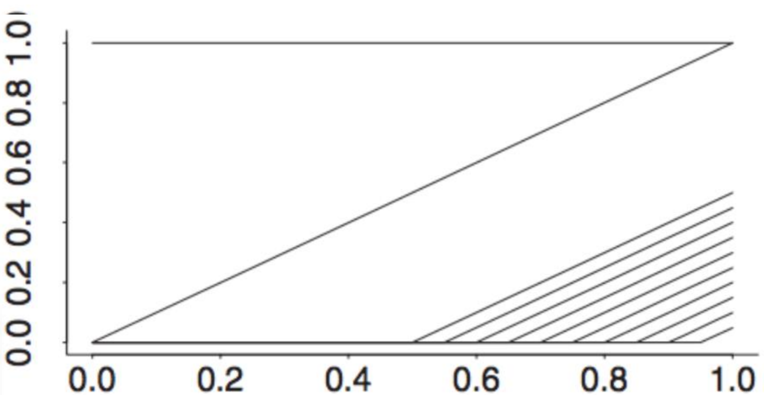
Truncated Linear Spline



- Corresponding Basis:

$$\mathbf{X} = \begin{bmatrix} 1 & x_1 & (x_1 - 0.5)_+ & (x_1 - 0.55)_+ & \cdots & (x_1 - 0.95)_+ \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & (x_n - 0.5)_+ & (x_n - 0.55)_+ & \cdots & (x_n - 0.95)_+ \end{bmatrix}$$

$$\boxed{f(x) = \beta_0 + \beta_1 x + \sum_{k=1}^{K} b_k (x - \kappa_k)_+}$$



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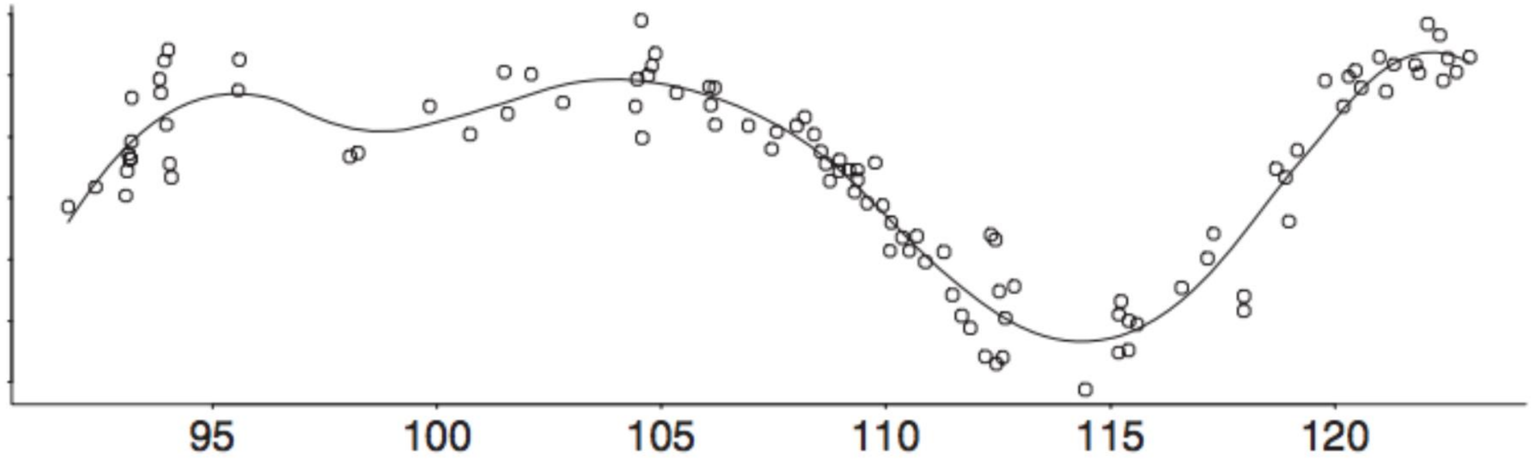
Truncated Power Spline



- Basis:

$$1, x, \ldots, x^p, (x-\kappa_1)_+^p, \ldots, (x-\kappa_k)_+^p,$$

- Model:

$$f(x) = \beta_0 + \beta_1 x + \cdots + \beta_p x^p + \sum_{k=1}^{p} \beta_{pk}(x-\kappa_k)_+^p.$$

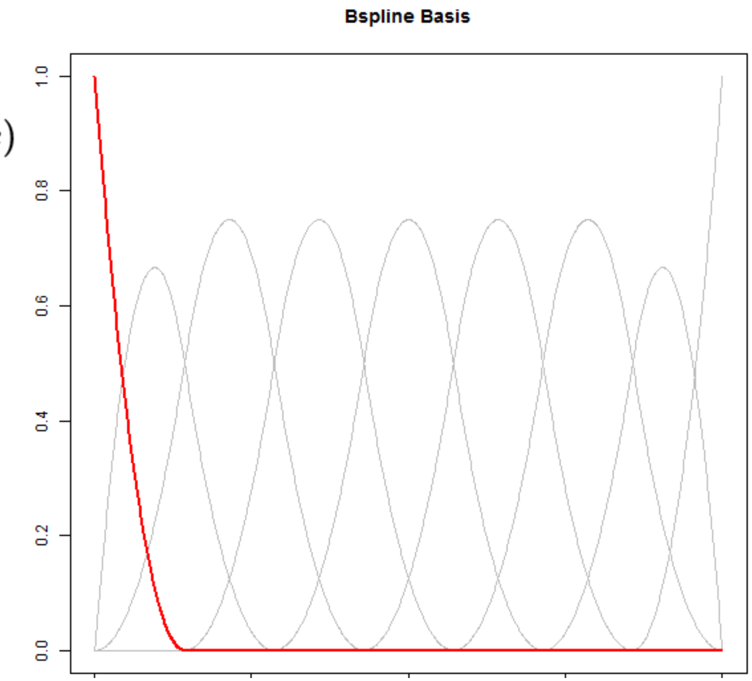
B-spline Bases

$$B_{i,0}(x) := \begin{cases} 1 & \text{if} \quad t_i \le x < t_{i+1} \\ 0 & \text{otherwise} \end{cases}$$

$$B_{i,k}(x) := \frac{x - t_i}{t_{i+k} - t_i} B_{i,k-1}(x) + \frac{t_{i+k+1} - x}{t_{i+k+1} - t_{i+1}} B_{i+1,k-1}(x)$$

Cox-de Boor recursion formula

$$\begin{array}{ccc}
 & & 0 \\
 & 0 & \\
0 & & B_{i-2,2} \\
 & B_{i-1,1} & \\
B_{i,0} & & B_{i-1,2} \\
 & B_{i,1} & \\
0 & & B_{i,2} \\
 & 0 & \\
 & & 0
\end{array}$$



Properties of B-splines

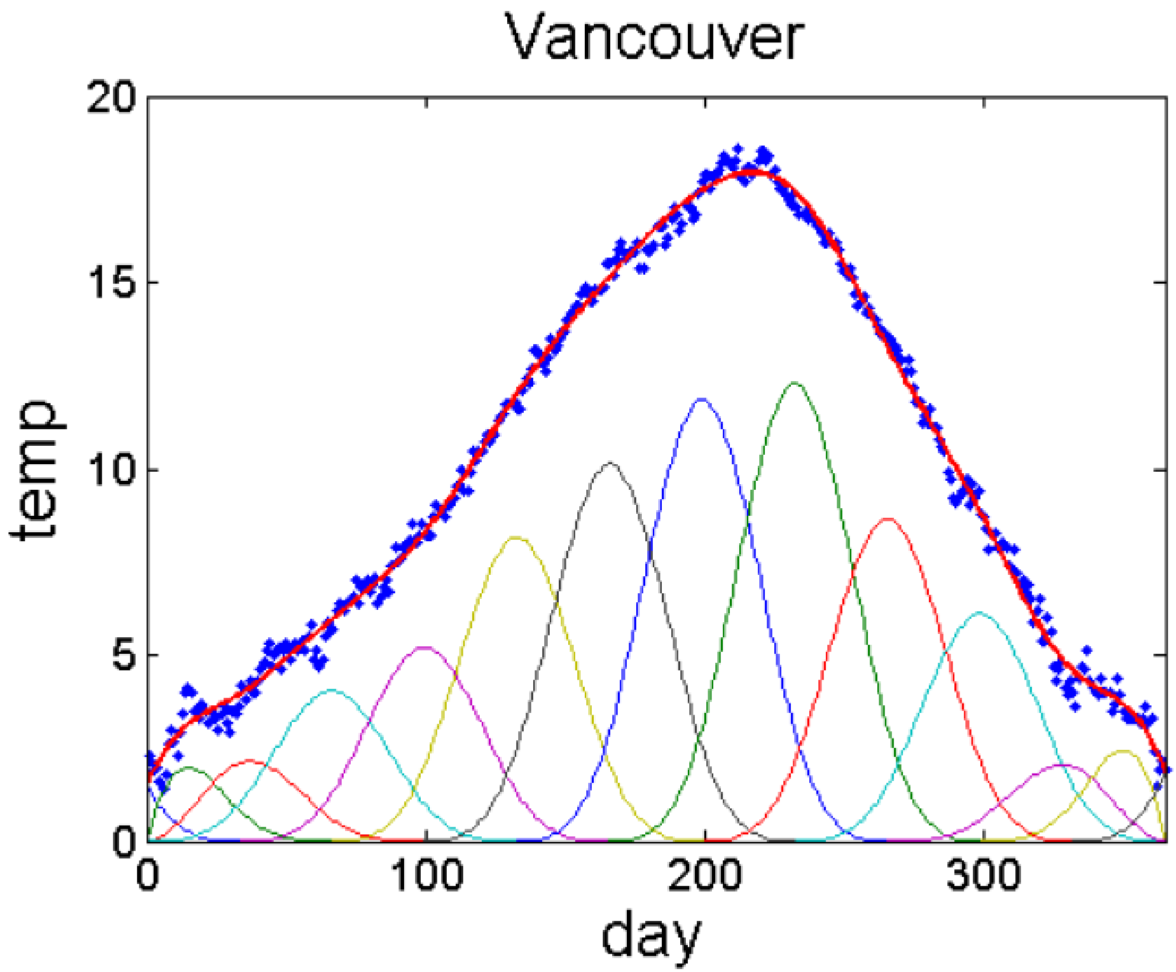
- Number of basis functions:

$$\textit{order} + \textit{number interior knots}$$

- Order m splines: derivatives up to $m - 2$ are continuous.
- Support on m adjacent intervals – highly sparse design matrix.

B-spline Bases

An illustration of basis expansions for *local* basis functions



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Other Bases in `fda` Library

Constant $\phi(t) = 1$, the simplest of all.

Monomial $1, x, x^2, x^3, \ldots,$ ..., mostly for legacy reasons.

Power $t^{\lambda_1}, t^{\lambda_2}, t^{\lambda_3}, \ldots$, powers are distinct but not necessarily integers or positive.

Exponential $e^{\lambda_1 t}, e^{\lambda_2 t}, e^{\lambda_3 t}, \ldots$

Other possible bases to represent $x(t)$:

Wavelets especially for sharp, local features (not in `fda`)

Empirical functional Principal Components (special topics)

1. Basis Expansions

Multi(Bi)variate Case

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From 1D to 2D Basis Functions using Tensor Product

- Suppose for each dimension we have a basis of function

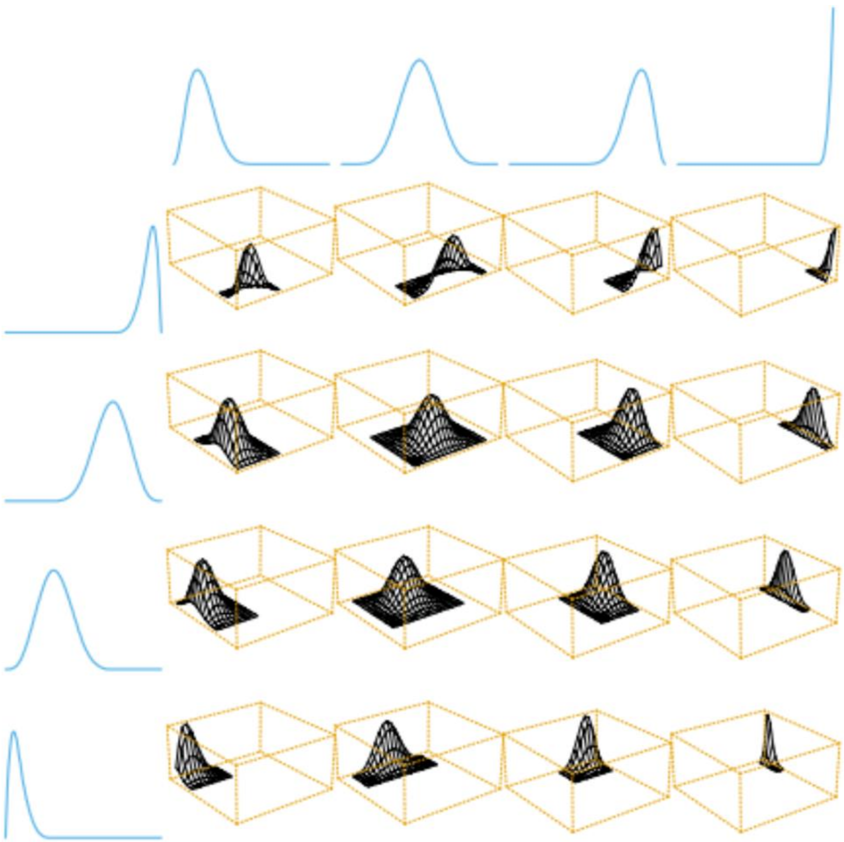
- We can write

$$f(x,y) = \sum_{i=1}^{N}\sum_{j=1}^{M} c_{ij}\phi_i(x)\psi_j(y)$$

- The $M \times N$ dimensional ***tensor product basis*** is:

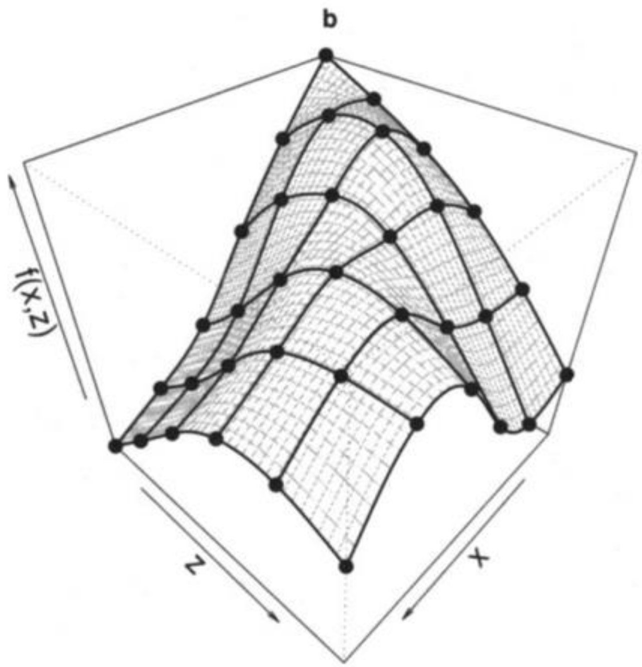
$$B = B_x \otimes B_y$$

- R code



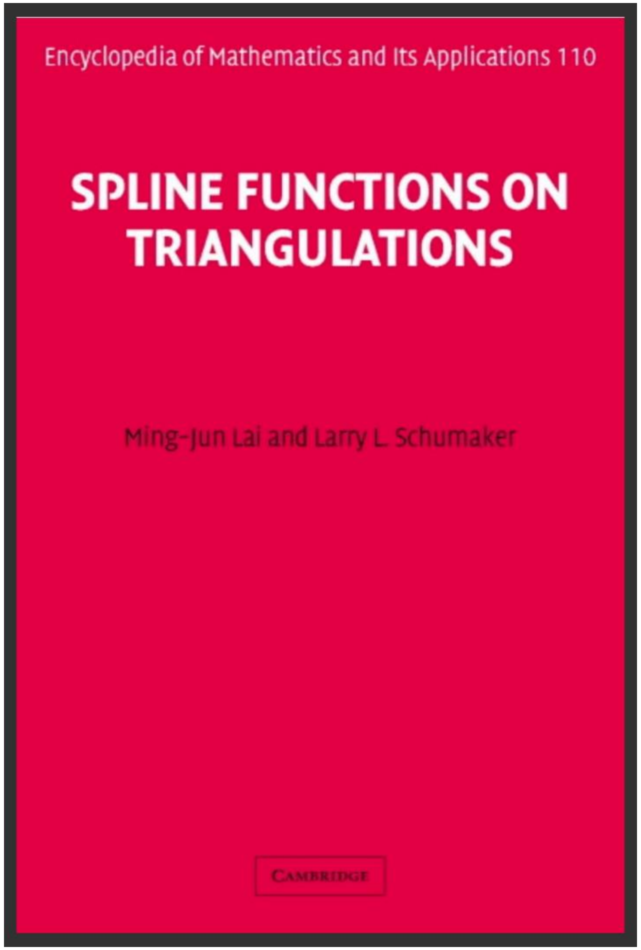
From Hastie, Tibshirani, Friedman book

Tensor Product: How it works



$$\begin{bmatrix} a_{1,1} & a_{1,2} \\ a_{2,1} & a_{2,2} \end{bmatrix} \otimes \begin{bmatrix} b_{1,1} & b_{1,2} \\ b_{2,1} & b_{2,2} \end{bmatrix} = \begin{bmatrix} a_{1,1} \begin{bmatrix} b_{1,1} & b_{1,2} \\ b_{2,1} & b_{2,2} \end{bmatrix} & a_{1,2} \begin{bmatrix} b_{1,1} & b_{1,2} \\ b_{2,1} & b_{2,2} \end{bmatrix} \\ & \\ a_{2,1} \begin{bmatrix} b_{1,1} & b_{1,2} \\ b_{2,1} & b_{2,2} \end{bmatrix} & a_{2,2} \begin{bmatrix} b_{1,1} & b_{1,2} \\ b_{2,1} & b_{2,2} \end{bmatrix} \end{bmatrix}$$

Triangulation and Spline

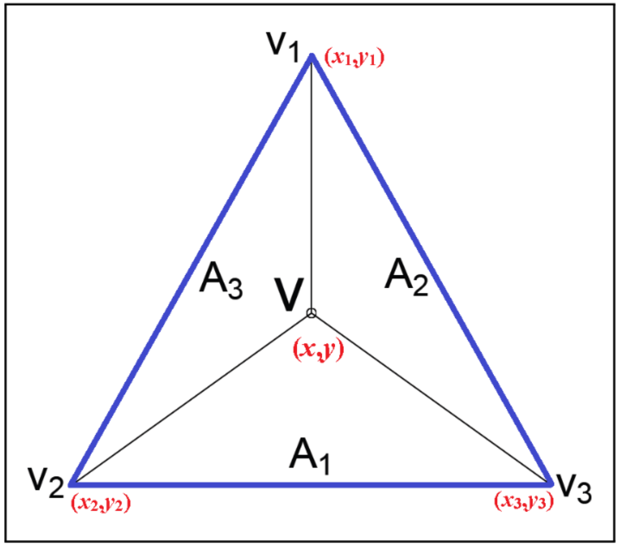


Triangulation

- Barycentric coordinates: Given a triangle A, any point $v \in \mathbb{R}^2$ can be written as

$$v = b_1 v_1 + b_2 v_2 + b_3 v_3,$$

where (b_1, b_2, b_3) is the barycentric coordinates of v with respect to A



- Some facts:
  - $b_1 + b_2 + b_3 = 1$
  - $b_i = \dfrac{\text{Area of } A_i}{\text{Area of } A}, \quad i = 1, 2, 3$
  - $v \in A \iff b_i \geq 0, \quad i = 1, 2, 3$

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Triangulation (Bivariate B–splines Basis)

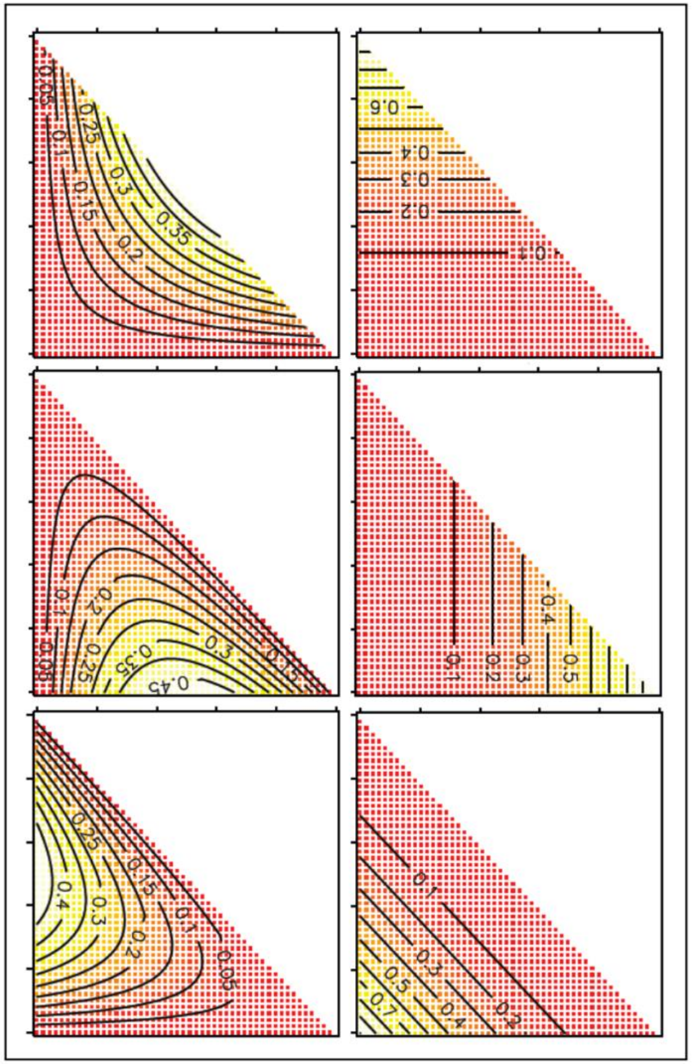
- Bivariate B—splines: Given a triangle A and a point $v \in A$, define:

$$B_{d,ijk}(v) := \frac{d!}{i!j!k!} b_1^i b_2^j b_3^k, \qquad i+j+k=d$$

- For a given triangle A and $d = 2$, B_d contains six functions (see right panel):

- B_d is a basis for $P_d(A)$: $\forall g \in P_d(A)$, $\exists c_{ijk}$:

$$g(v) = \sum_{i+j+k=d} c_{ijk} B_{d,ijk}(v)$$



Triangulation (Smoothness conditions)

Theorem

Suppose there are two triangles A_1 and A_2 sharing edge e. ω is any direction not parallel to common edge e and $D^n_\omega p(v)$ is nth order derivative in direction ω at point v. Then

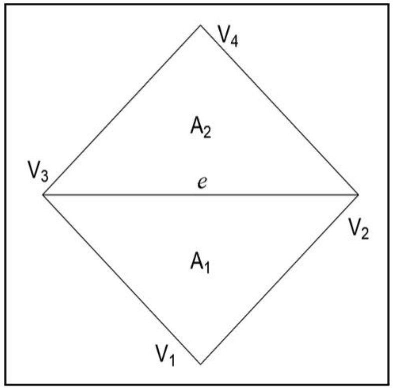
$$D^\ell_\omega p_1(v) = D^\ell_\omega p_2(v), \quad \forall v \in e \text{ and } \ell = 0, \cdots, r \quad \textit{iff}$$

$$c^{(2)}_{ijk} = \sum_{\nu+\mu+\kappa=\ell} c^{(1)}_{\nu,k+\mu,j+\kappa} B^{(1)n}_{\nu\mu\kappa}(v_4), \quad j+k = d-\ell, \; \ell = 0, \cdots, r.$$

- Hint: $\mathbf{A}\mathbf{c} = 0$ is the linear constraint for smoothness of the boundaries

  $$\Downarrow$$

  spanning set for the null space of $\mathbf{A}$ is a basis that satisfies the constraint



R code

Summary

1. Basis expansions: just like adding different independent variables in linear regression
2. Monomial basis: direct extension of adding interaction and quadratic terms. Poor numerics, bad for derivatives.
3. Fourier basis: classical, common in signal processing etc. Great for periodic functions. Must be infinitely differentiable.
4. B-spline basis: locally polynomial. Allows control of smoothness and accuracy. Local definition $\Rightarrow$ good numerics.
5. Other basis systems also exist.
6. What is best depends on the data.
   - The order of the spline should be at least $k+2$ if you are interested in k derivatives.
   - Place more knots where you know there is strong curvature, and fewer where the function changes slowly.
   - Be sure there is at least one data point in every interval.
   - Knots are often equally spaced (a useful default)
   - Later, we'll discuss placing a knot at each point of observation.

2. Smoothing Penalties

Univariate Case

Ordinary Least-Squares Estimates

Assume we have observations for a single curve

$$y_i = x(t_i) + \epsilon$$

and we want to estimate

$$x(t) \approx \sum_{j=1}^{K} c_j \phi_j(t)$$

Minimize the sum of squared errors:

$$SSE = \sum_{i=1}^{n} (y_i - x(t_i))^2 = \sum_{i=1}^{n} (y_i - \Phi(t_i)\mathbf{c})^2$$

This is just linear regression!

Linear Regression on Basis Functions

- If the N by K matrix $\mathbf{\Phi}$ contains the values $\phi_j(t_k)$, and $\mathbf{y}$ is the vector $(y_1, \ldots, y_N)$, we can write

$$SSE(\mathbf{c}) = (\mathbf{y} - \mathbf{\Phi}\mathbf{c})^T(\mathbf{y} - \mathbf{\Phi}\mathbf{c})$$

- The error sum of squares is minimized by the *ordinary least squares estimate*

$$\hat{\mathbf{c}} = \left(\mathbf{\Phi}^T\mathbf{\Phi}\right)^{-1}\mathbf{\Phi}^T\mathbf{y}$$

- Then we have the estimate

$$\hat{x}(t) = \Phi(t)\hat{\mathbf{c}} = \Phi(t)\left(\mathbf{\Phi}^T\mathbf{\Phi}\right)^{-1}\mathbf{\Phi}^T\mathbf{y}$$

The Standard Model for Residual Distribution

- least squares is optimal for residuals that are independently and identically normal with mean 0 and variance σ.
- That is

$$E\mathbf{y} = \mathbf{\Phi c} \text{ and } \mathrm{Var}\left[\mathbf{y}\right] = \sigma^2 \mathbf{I}$$

- Call this the *standard model* for the distribution of residuals.
- An unbiassed estimate is

$$\hat{\sigma}^2 = \frac{1}{N-K} MSSE$$

- We know that $\hat{\mathbf{c}} = \left(\mathbf{\Phi}^T \mathbf{\Phi}\right)^{-1} \mathbf{\Phi}^T \mathbf{y} = C\mathbf{y}$
- Then under the standard model

$$\mathrm{Var}\left[\hat{\mathbf{c}}\right] = \sigma^2 C I C^T = \sigma^2 \left(\mathbf{\Phi}^T \mathbf{\Phi}\right)^{-1}$$

The Standard Model for Residual Distribution

- Then we have the estimate

$$\hat{x}(t) = \Phi(t)\hat{\mathbf{c}} = \Phi(t)\left(\boldsymbol{\Phi}^T\boldsymbol{\Phi}\right)^{-1}\boldsymbol{\Phi}^T\mathbf{y}$$

When we look at the values of $\hat{x}$ at the observation points we have

$$\hat{\mathbf{y}} = \boldsymbol{\Phi}\left(\boldsymbol{\Phi}^T\boldsymbol{\Phi}\right)^{-1}\boldsymbol{\Phi}^T\mathbf{y} = S\mathbf{y}$$

S is referred to as the *smoothing matrix.*

- And the variance-covariance matrix of the fitted values is

$$\mathrm{Var}\left[\hat{\mathbf{y}}\right] = \boldsymbol{\Phi} C \Sigma C^T \boldsymbol{\Phi}^T = \sigma^2 S$$

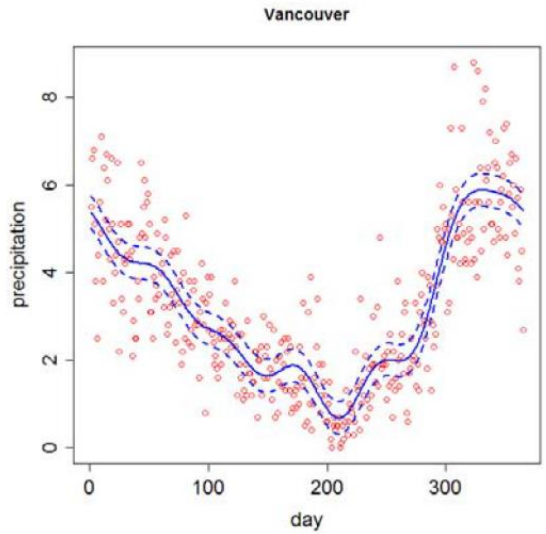
Pointwise Confidence Bands

- For each point we calculate lower and upper bands for $\hat{y}(t)$ by

$$\hat{y}(t) \pm 2\sqrt{\mathrm{Var}\left[\hat{y}(t)\right]}$$

- These bands are not confidence bands for the entire curve, but only for the value of the curve at a fixed point.
- Ignores bias in the estimated curve

Fitted Vancouver Precipitation Data with 13 Fourier Bases



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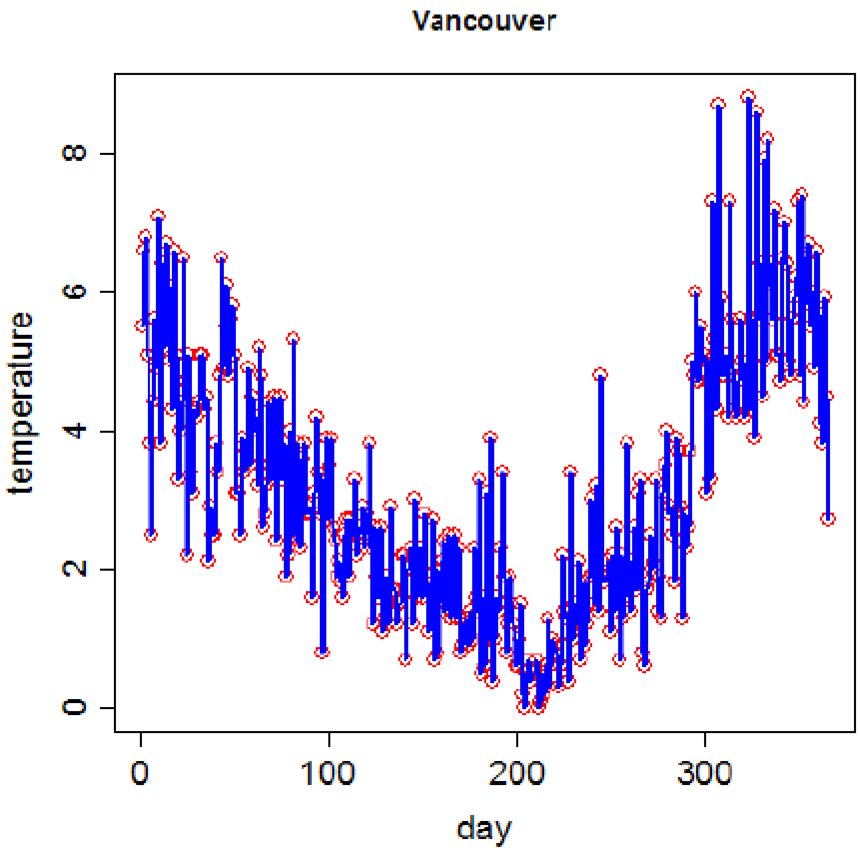
Choosing the Number of Basis Functions

Vancouver Precipitation: 365 Fourier Bases



- Too many basis functions over-fits the data and reflect errors of measurement
- Too few basis functions fails to capture interesting features of the curves.

Cross-Validation

One method of choosing a model:

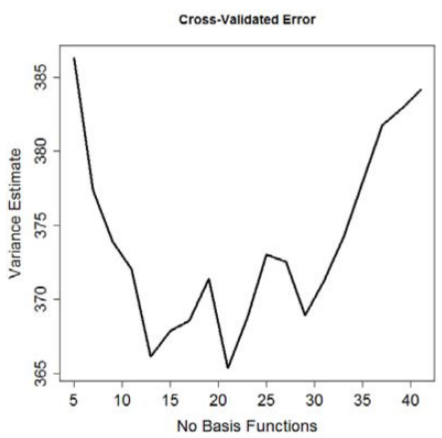
- leave out one observation (t_i, y_i)
- estimate $\hat{x}_{-i}(t)$ from remaining data
- measure $y_i - \hat{x}_{-i}(t)$
- Choose K to minimize the *ordinary cross-validation* score:

$$\mathrm{OCV}\left[\hat{x}\right] = \sum \left(y_i - \hat{x}_{-i}(t_i)\right)^2$$

- for a linear smooth $\hat{y} = Sy$,

$$\mathrm{OCV}\left[\hat{x}\right] = \sum \frac{\left(y_i - \hat{x}(t_i)\right)^2}{(1 - s_{ii})^2}$$

Cross Validation for Vancouver Precipitation



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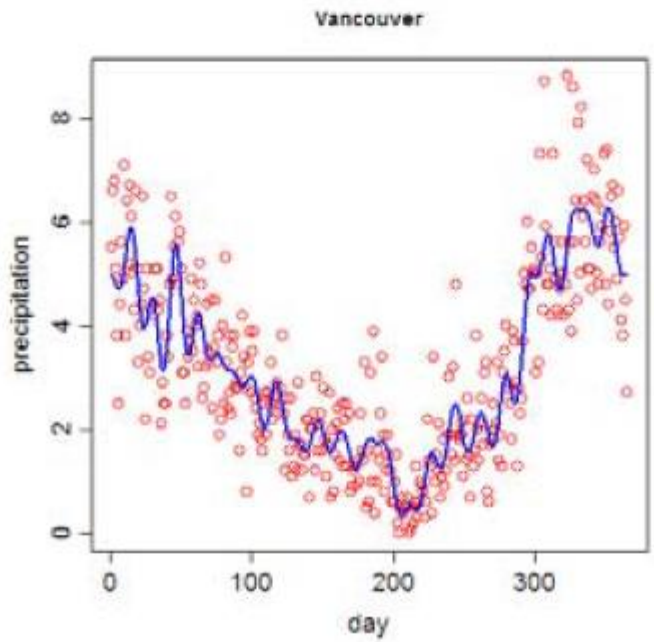
What do we mean by smoothness?

Some things are fairly clearly smooth:

- constants
- straight lines

What we really want to do is eliminate small "wiggles" in the data.



The D Operator

We use the notation that for a function $x(t)$,

$$Dx(t) = \frac{d}{dt}x(t)$$

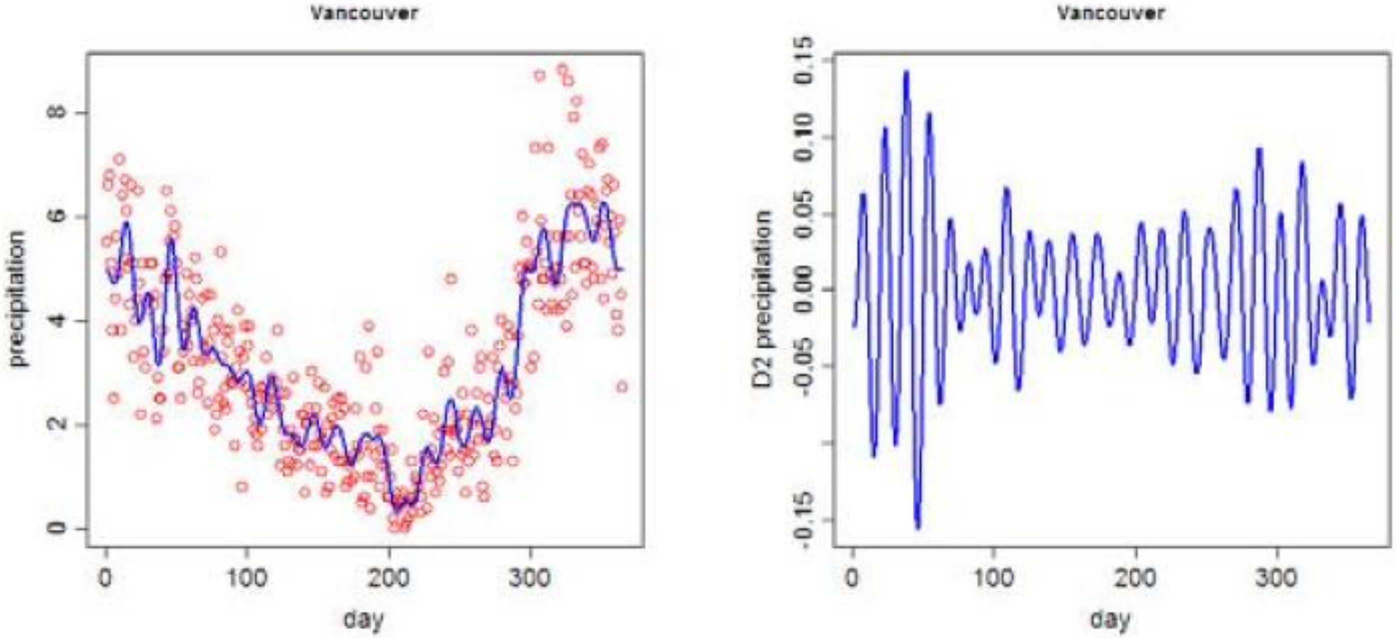
We can also define further derivatives in terms of powers of D:

$$D^2x(t) = \frac{d^2}{dt^2}x(t), \ldots, D^kx(t) = \frac{d^k}{dt^k}x(t), \ldots$$

- $Dx(t)$ is the instantaneous *slope* of $x(t)$; $D^2x(t)$ is its *curvature*.

Curvature of Vancouver Precipitation

53 Fourier bases:



The D Operator

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- $Dx(t)$ is the instantaneous *slope* of $x(t)$; $D^2x(t)$ is its *curvature*.
- We measure the size of the curvature for all of f by

$$J_2(x) = \int \left[D^2x(t)\right]^2 dt$$

Smoothing Penalties

- Problem: how to choose a basis? Large affect on results.
- Finesse this by specifying a very rich basis, but then imposing smoothness.
- In particular, add a penalty to the least-squares criterion:

$$\text{PENSSE} = \sum_{i=1}^{n} (y_i - x(t_i))^2 + \lambda J[x]$$

- $J[x]$ measures "roughness" of x.
- λ represents a continuous tuning parameter (to be chosen):
  - $\lambda \uparrow \infty$: roughness increasingly penalized ,$x(t)$ becomes smooth.
  - $\lambda \downarrow 0$: penalty reduces, $x(t)$ fits data better.

The Smoothing Spline Theorem

Consider the "usual" penalized squared error:

$$PENSSE_{\lambda}(x) = \sum (y_i - x(t_i))^2 + \lambda \int \left[D^2 x(t)\right]^2 dt$$

- The function $x(t)$ that minimizes $PENSSE_{\lambda}(x)$ is
  - a spline function of order 4 (piecewise cubic)
  - with a knot at each sample point t_i

Cubic B-splines are exact; other systems will approximate solution as close as desired.

Calculating the Penalized Fit

When $x(t) = \Phi(t)\mathbf{c}$, we have that

$$\int \left[D^2 x(t)\right]^2 dt = \int \mathbf{c}^T \left[D^2\Phi(t)\right] \left[D^2\Phi(t)\right]^T \mathbf{c} dt = \mathbf{c}^T R_2 \mathbf{c}$$

$[R_2]_{jk} = \int [D^2\phi_j(t)][D^2\phi_k(t)]dt$ is the *penalty matrix*.

The penalized least squares estimate for $\mathbf{c}$ is n

$$\hat{\mathbf{c}} = \left[\mathbf{\Phi}^T\mathbf{\Phi} + \lambda R_2\right]^{-1} \mathbf{\Phi}^T\mathbf{y}$$

This is still a linear smoother:

$$\hat{\mathbf{y}} = \mathbf{\Phi}\left[\mathbf{\Phi}^T\mathbf{\Phi} + \lambda R_2\right]^{-1} \mathbf{\Phi}^T\mathbf{y} = S(\lambda)\mathbf{y}$$

How about a simpler penalty?

- Up to mid-1990's O'Sullivan penalty was very popular, where

➢ $S(x) = \sum_{i=1}^{n}\left\{y_i - \sum_{j=1}^{M} c_j \Phi_j(x)\right\}^2 + \lambda \int_{x_{\min}}^{x_{\max}}\left\{\sum_{j=1}^{M} c_j \Phi_j''(x)\right\}^2$

- Then Eilers/Marx proposed a penalty based on finite difference (Pspline), where

➢ $S(x) = \sum_{i=1}^{n}\left\{y_i - \sum_{j=1}^{M} c_j \Phi_j(x)\right\}^2 + \lambda \sum_{j=k+1}^{M}\left(\Delta_k c_j\right)^2$

where

– $\Delta_k c_j = c_j - c_{j-1}$ and

– $\Delta_k = \Delta(\Delta_{k-1})$

More on PSpline

- We may write the difference functions Δ_k into a matrix form, D_k. For example, for $k = 1$ we have
  - $D_1 = \begin{bmatrix} 1 & -1 & 0 & \cdots & 0 \\ 0 & 1 & -1 & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & -1 & 1 \end{bmatrix}_{(M-1 \times M)}$
- The positive definite matrix that controls the smoothness has the following quadratic form $R_1 = D_1^T D_1$, where

$$D_1^{\mathsf{T}} D_1 = \begin{pmatrix} 1 & -1 & 0 & \cdots & 0 & 0 \\ -1 & 2 & -1 & \cdots & 0 & 0 \\ 0 & -1 & 2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2 & -1 \\ 0 & 0 & 0 & \cdots & -1 & 1 \end{pmatrix}$$

Linear Smooths and Degrees of Freedom

- In least squares fitting, the degrees of freedom used to smooth the data is exactly K, the number of basis functions

- In penalized smoothing, we can have $K > n$.

- The smoothing penalty reduces the flexibility of the smooth

- The degrees of freedom are controlled by λ. A natural measure turns out to be

$$df(\lambda) = \text{trace}\left[S(\lambda)\right], \; S(\lambda) = \mathbf{\Phi}\left[\mathbf{\Phi}^T\mathbf{\Phi} + \lambda R_L\right]^{-1}\mathbf{\Phi}^T$$

Choosing Smoothing Parameters: Cross Validation

There are a number of data-driven methods for choosing smoothing parameters.

- Ordinary Cross Validation: leave one point out and see how well you can predict it:

$$\mathrm{OCV}(\lambda) = \frac{1}{n}\sum\left(y_i - x_\lambda^{-i}(t_i)\right)^2 = \frac{1}{n}\sum\frac{(y_i - x_\lambda(t_i))^2}{(1 - S(\lambda)_{ii})^2}$$

- Generalized Cross Validation tends to smooth more:

$$\mathrm{GCV}(\lambda) = \frac{\sum(y_i - x_\lambda(t_i))^2}{[\mathrm{trace}(\mathbb{I} - S(\lambda))]^2}$$

  will be used here.
- Other possibilities: AIC, BIC,...

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Constrained Functions

There are some situations in which we want to include known restrictions about $x(t)$.

- $x(t)$ is always positive

$$x(t) = e^{W(t)}$$

- $x(t)$ is always increasing (or decreasing)

$$Dx(t) = e^{W(t)} \quad \xrightarrow{Dx(t) > 0} \quad x(t) = \alpha + \int_{t_0}^{t} e^{W(s)} ds$$

- $x(t)$ is a density

$x(t)$ a density $\Rightarrow$ positive, integrates to 1 $\longrightarrow$ $$x(t) = e^{W(t)} \Big/ \int e^{W(t)} dt$$

Idea: Enforce these conditions by transforming $x(t)$.

$$\text{Define } W(t) = \Phi(t)\mathbf{c}$$

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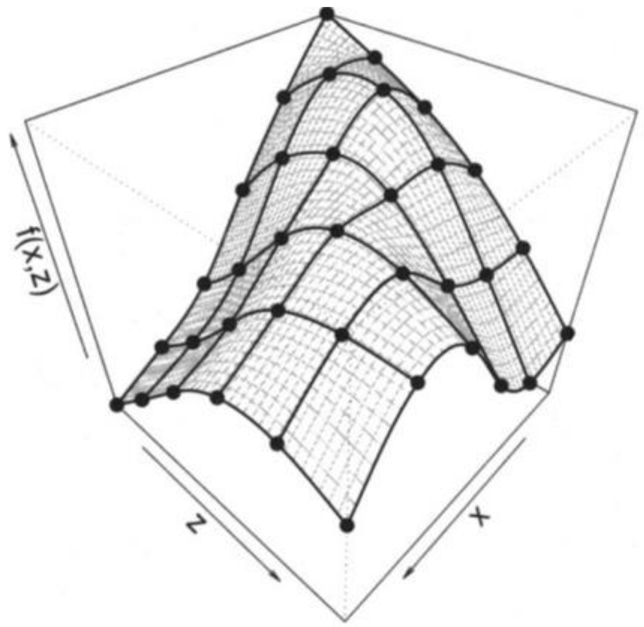
2. Smoothing Penalties

Multi(Bi)variate Case

Tensor product: Penalty

- $\boldsymbol{R} = [I_N \otimes R^x + R^y \otimes I_M]$, where
  - $R^x = \{D_k^x\}^T D_k^x$ and
  - $R^y = \{D_k^y\}^T D_k^y$
- This can be generalized to higher dimensions, e.g. in 3D case:
- $\boldsymbol{R}$ has three associated penalties, R^j ($c^T R_j c$), where
  - $R^j = \{\widetilde{D}_k^j\}^T \widetilde{D}_k^j$ and
  - $\widetilde{D}_k^1 = D_k^1 \otimes I_N \otimes I_O$
  - $\widetilde{D}_k^2 = I_M \otimes D_k^2 \otimes I_O$
  - $\widetilde{D}_k^3 = I_M \otimes I_N \otimes D_k^3$



Triangulation Basis: The thin-plate Penalty

- The thin-plate penalty (Green and Silverman, 1994):

$$\mathrm{PEN}(g) = \iint (g_{11}^2 + 2g_{12}^2 + g_{22}^2)\, dx_1 dx_2$$

  where

  – $g_{ij}(x_1, x_2) = \frac{\partial g(x_1,x_2)}{\partial x_i \partial x_j}, \qquad i,j = 1,2$

- Let $g(\boldsymbol{x}) = \boldsymbol{\phi}(\boldsymbol{x})^T c$, and
- $\boldsymbol{\phi}_{ij}(\boldsymbol{x}) = \left(\phi_{1,ij}(\boldsymbol{x}), \cdots, \phi_{L,ij}(\boldsymbol{x})\right)^T$ be the vector of partial derivatives: $g_{ij}(\boldsymbol{x}) = \boldsymbol{\phi}_{ij}(\boldsymbol{x})^T c$
- The penalty function can be written in quadratic form as
  – $\mathrm{PEN}(g) = c^T \boldsymbol{R} c$, where
  – $\boldsymbol{R} = \iint \{\boldsymbol{\phi}_{11}(\boldsymbol{x})\boldsymbol{\phi}_{11}(\boldsymbol{x})^T + 2\boldsymbol{\phi}_{12}(\boldsymbol{x})\boldsymbol{\phi}_{12}(\boldsymbol{x})^T + \boldsymbol{\phi}_{22}(\boldsymbol{x})\boldsymbol{\phi}_{22}(\boldsymbol{x})^T\} d\boldsymbol{x}$

3. Further Exploration of the Functional Data

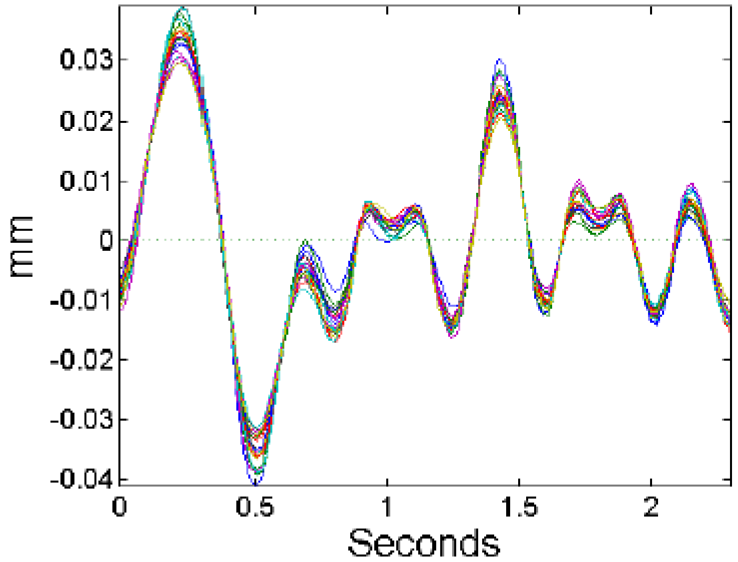
Dimension Reduction

Exploring Functional Data

How do we understand

1. mean
2. variance
3. covariance
4. important parts of covariance

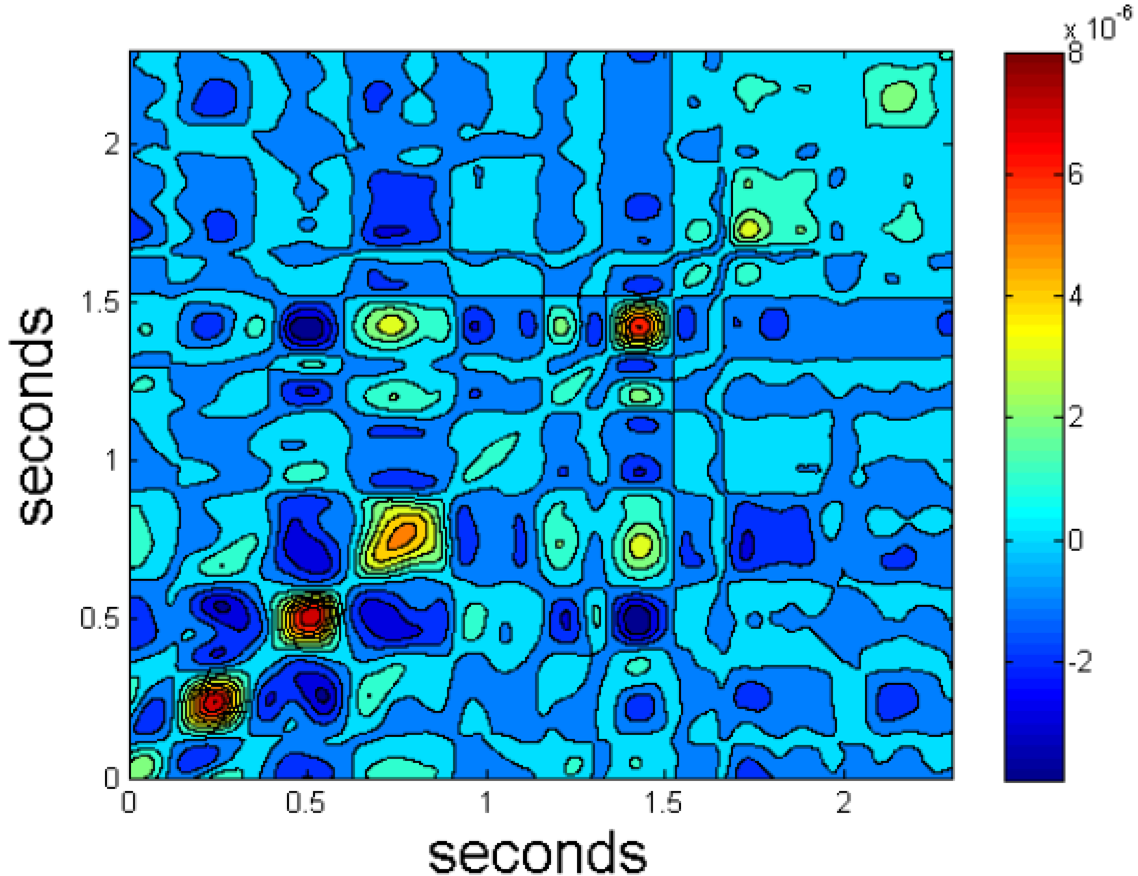
in functional data?



The Covariance Surface

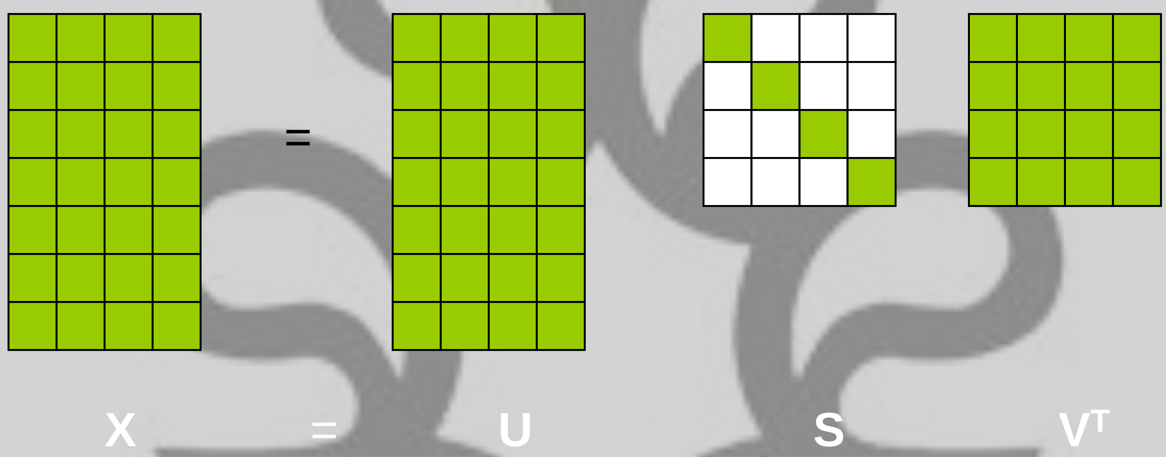
The covariance between $x(s)$ and $x(t)$ is a *surface*

$$C(s,t) = \frac{1}{n-1}\sum (x_i(s) - \bar{x}(s))(x_i(t) - \bar{x}(t))$$



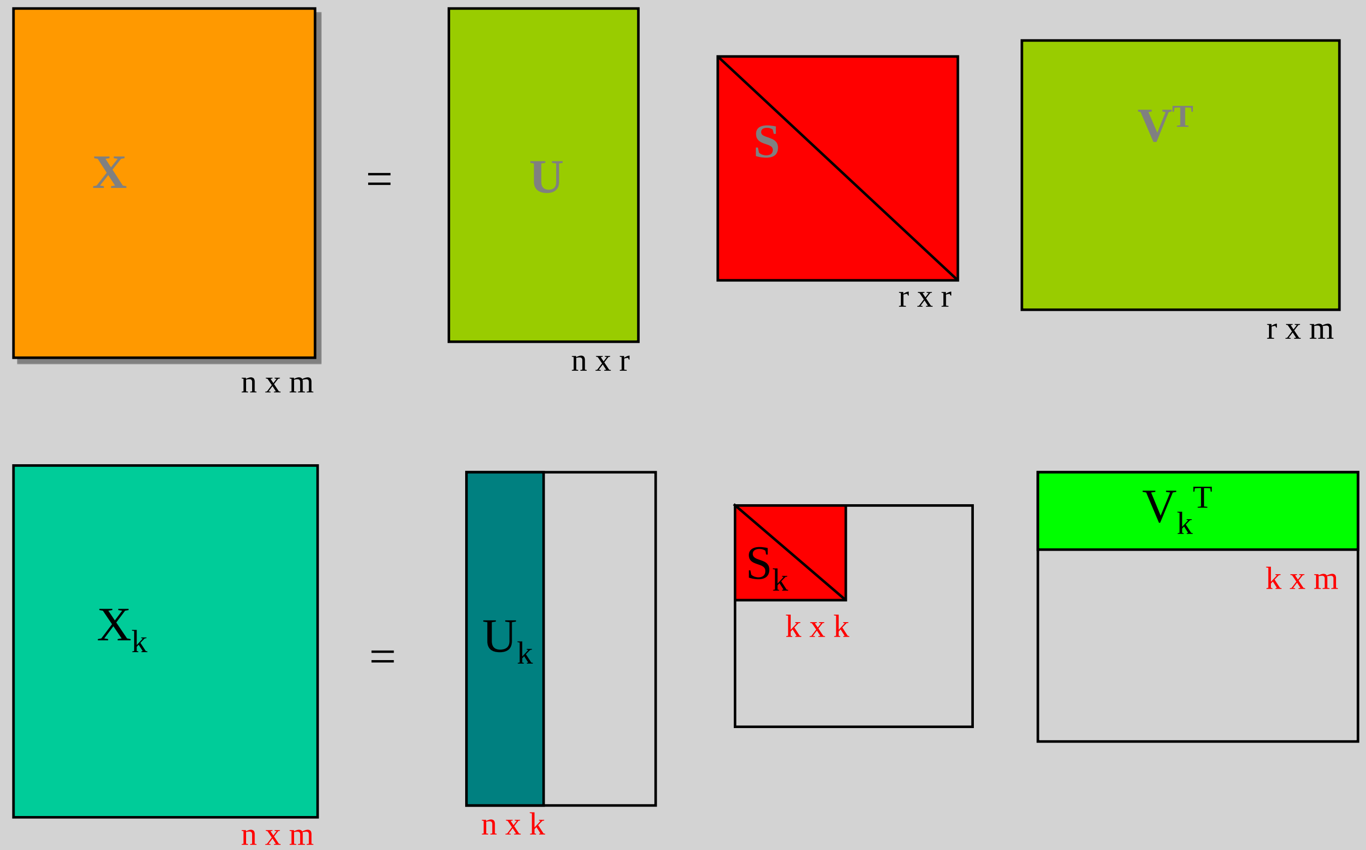
Singular Value Decomposition(SVD)

SVD of a Matrix



U and ***V*** are orthogonal matrices, and ***S*** is a diagonal matrix consisting of singular values.

Truncated Singular Value Decomposition (TSVD)



The reconstructed matrix $X_k = U_k.S_k.V_k^T$ is the closest *rank-k* matrix to the original matrix *X*.

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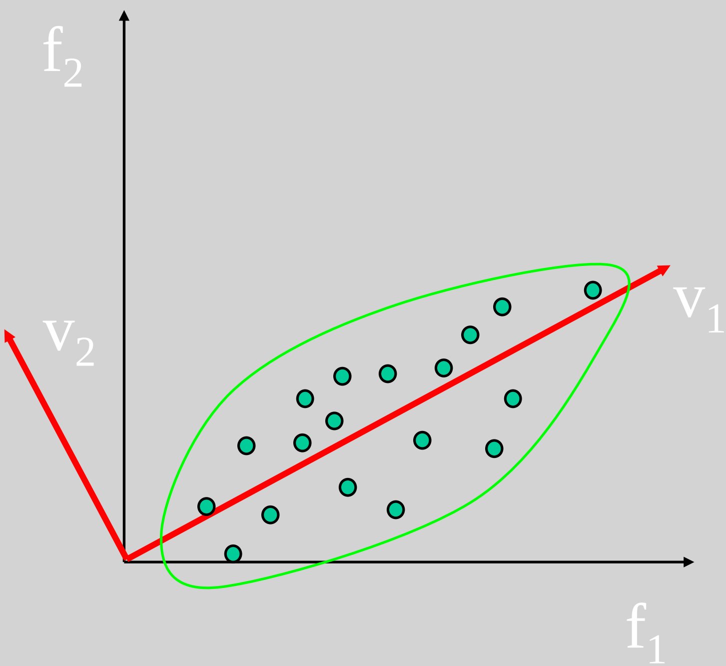
Geometric Interpretation of PCA

- Intuition: find the axis that shows the greatest variation, and project all points into this axis



•$\underset{v}{\operatorname{argmax}}\ Var(v^T X_r) = \underset{v}{\operatorname{argmax}}\ v^T\, Var(X_r) v$

But note that the sample covariance is given by $S=n^{(-1)}(X^TX)$. Hence

We want to find the direction ***v*** such that:

•$\underset{v}{\operatorname{argmax}}\ v^T(X^TX)v = \underset{v}{\operatorname{argmax}}\ ||Xv||_2$

•It can be shown that ***v*** is the eigenvector associated to the largest eigenvalue of X^TX

Connection between SVD and Eigen Decomposition

SVD of a Matrix: observations

$$X = U\,S\,V^T$$

Multiply both sides by X^T

Multiplying on the left

$X^TX = (U\,S\,V^T)^T\,U\,S\,V^T$

$X^TX = (V\,S\,U^T)\,U\,S\,V^T$

remember $U^TU = I$

$X^TX = V\,S^2\,V^T$

Multiplying on the right

$XX^T = U\,S\,V^T\,(U\,S\,V^T)^T$

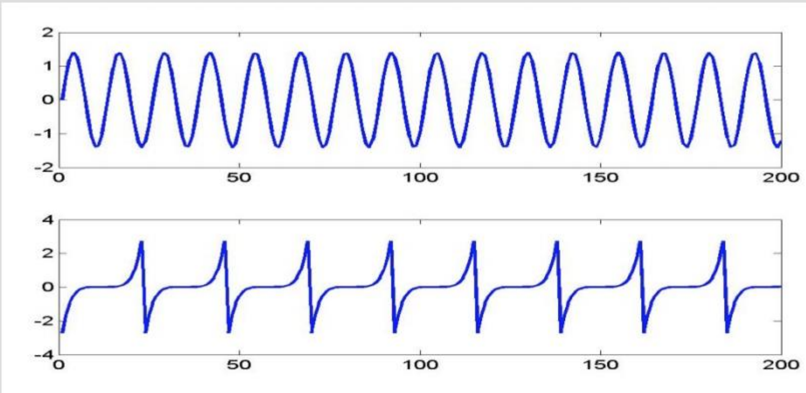
$XX^T = U\,S\,V^T\,(V\,S\,U^T)$

$V^TV = I$

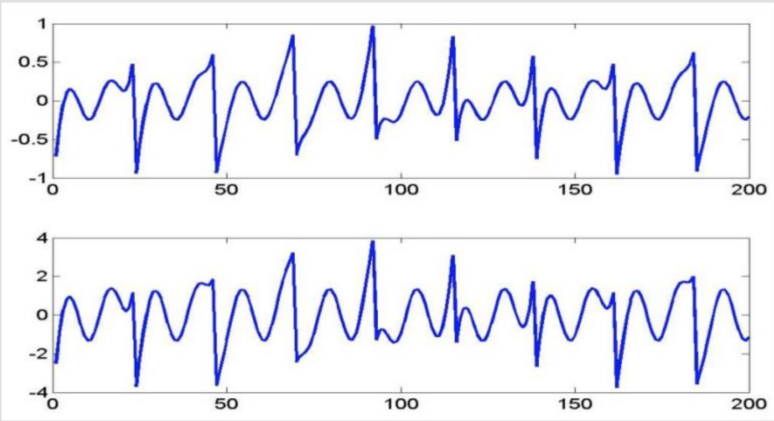
$XX^T = U\,S^2\,U^T$

$U = X\,V\,S^{-1}$

Independent Component Analysis (ICA)



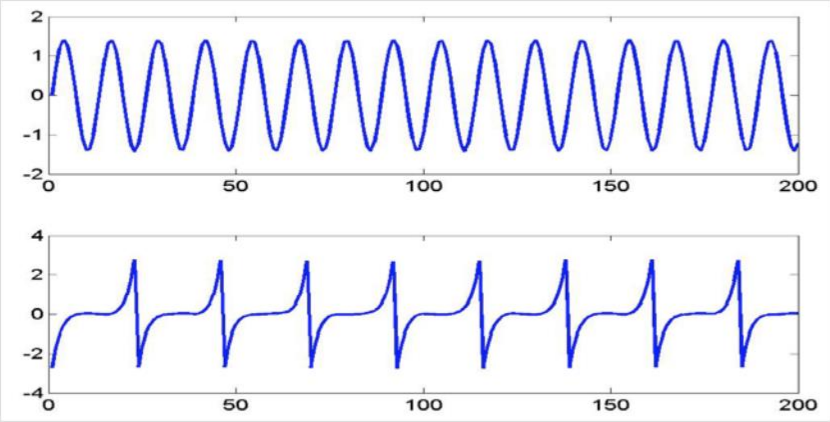
original signals



Observations (Mixtures)

$$
\begin{aligned}
x_1(t) &= a_{11}s_1(t) + a_{12}s_2(t) \\
x_2(t) &= a_{21}s_1(t) + a_{22}s_2(t)
\end{aligned}
$$

Model



ICA estimated signals

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Independent Component Analysis (ICA)

We observe

$$\begin{pmatrix} x_1(1) \\ x_2(1) \end{pmatrix}, \begin{pmatrix} x_1(2) \\ x_2(2) \end{pmatrix}, \ldots, \begin{pmatrix} x_1(t) \\ x_2(t) \end{pmatrix}$$

Model

$$\begin{aligned} x_1(t) &= a_{11}s_1(t) + a_{12}s_2(t) \\ x_2(t) &= a_{21}s_1(t) + a_{22}s_2(t) \end{aligned}$$

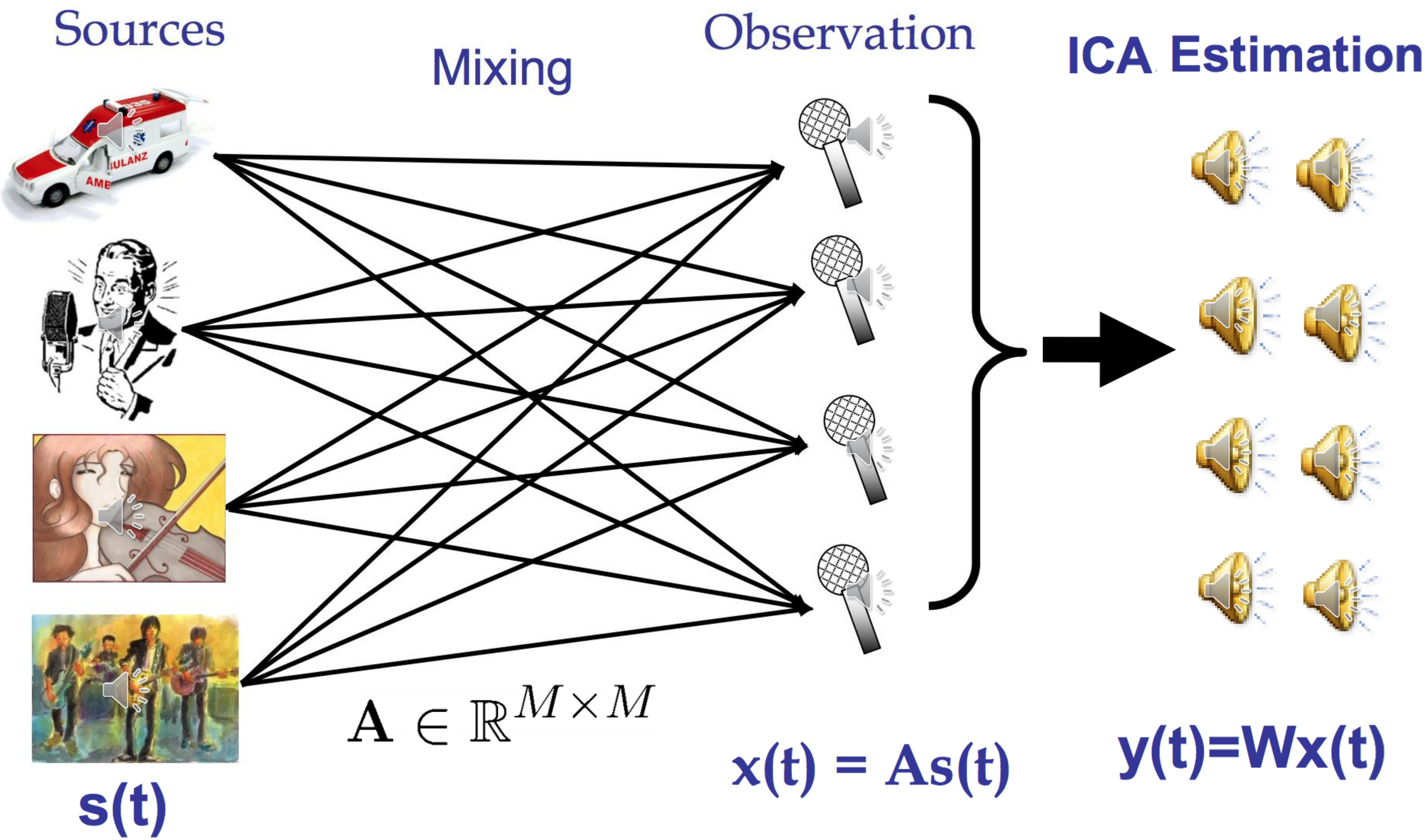
We want

$$\begin{pmatrix} s_1(1) \\ s_2(1) \end{pmatrix}, \begin{pmatrix} s_1(2) \\ s_2(2) \end{pmatrix}, \ldots, \begin{pmatrix} s_1(t) \\ s_2(t) \end{pmatrix}$$

But we don't know $\{a_{ij}\}$, nor $\{s_i(t)\}$

Goal: Estimate $\{s_i(t)\}$, (and also $\{a_{ij}\}$)

The Cocktail Party Problem



ICA vs PCA - Similarities

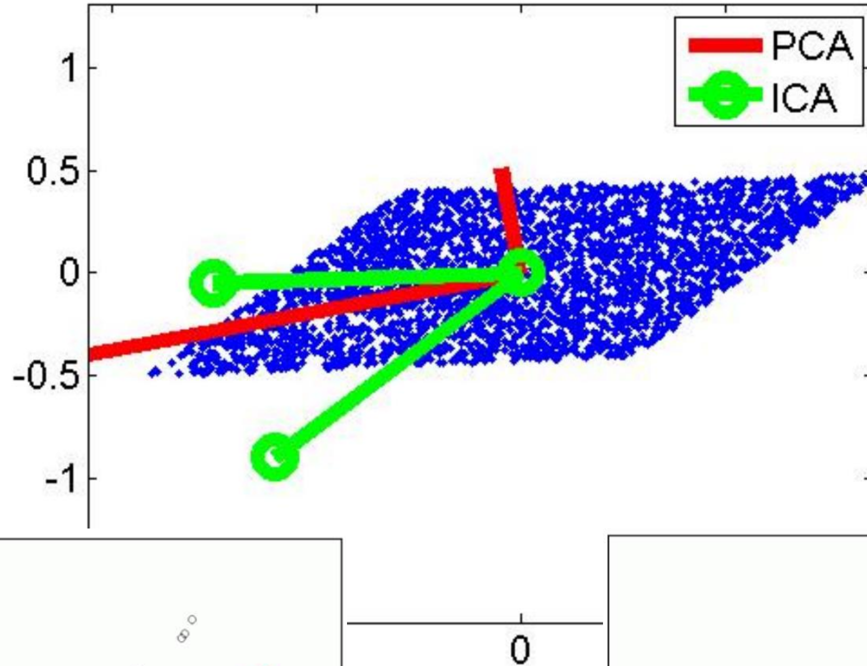
- PCA: $\mathbf{X} = \mathbf{US}$, where $\boldsymbol{S} = \boldsymbol{\Sigma}\mathbf{V}^{\mathbf{T}}$ and $\mathbf{U}^{\mathbf{T}}\mathbf{U} = \mathbf{I}$
- ICA: $\mathbf{X} = \boldsymbol{AS}$, where $\boldsymbol{A}$ is invertible

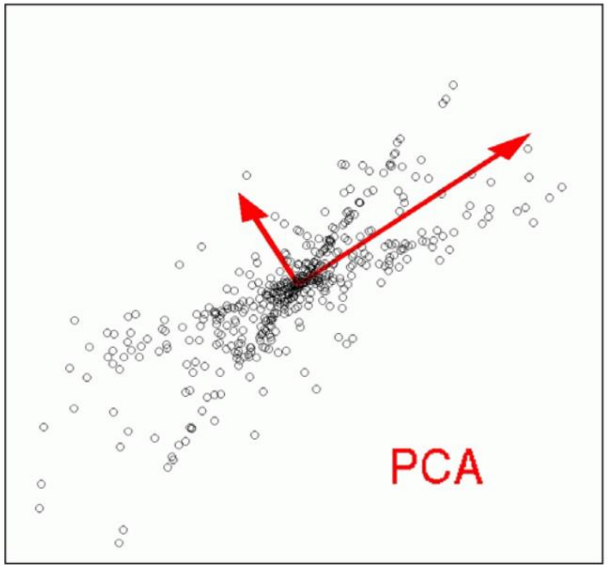
- PCA: just removes correlations, **not** higher order dependence
- ICA: removes correlations, **and** higher order dependence

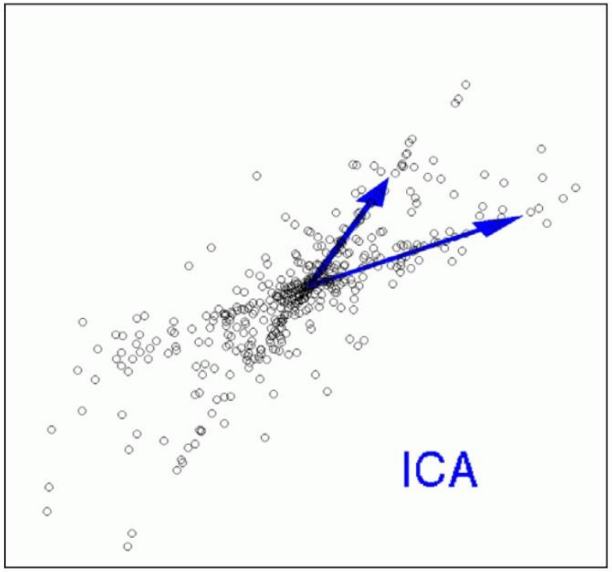
- PCA: Some components are **more important** than others
- ICA: Components are **equally important**

- PCA: vectors are orthogonal
- ICA: vectors are **not** orthogonal

ICA vs PCA – Cont…







The `fda` Package

fda Objects

The `fda` package provides utilities based on basis expansions and smoothing penalties.

`fda` works by defining objects that can be manipulated with pre-defined functions.

In particular

`basis` objects define basis systems that can be used

`fd` objects store functional data objects

`bifd` objects store functions of two-dimensions

`Lfd` objects define smoothing penalties

`fdPar` objects collect all three plus a smoothing parameter

Each of these are lists with prescribed elements.

Basis Objects

Define basis systems of various types. They have elements

- `rangeval` Range of values for which basis is defined.
- `nbasis` Number of basis functions.

Specific basis systems require other arguments.

Basis objects created by `create....basis` functions. eg

```
fbasis = create.fourier.basis(c(0,365),21)
```

creates a fourier basis on [0 365] with 21 basis functions.

Bspline Basis Objects

Bspline bases also require

- **norder** Order of the splines.
- **breaks** Knots (or break-points) for the splines.

```
nbasis = 17
norder = 6
months = cumsum(c(0,31,28,31,30,31,30,31,31,30,31,30,31))
bbasis = create.bspline.basis(c(0,365),nbasis,norder,months)
```

Creates a B-spline basis of order 6 on the year ([0 365]) with knots at the months.

Note that

$$\texttt{nbasis} = \texttt{length(knots)+norder-2}$$

`nbasis` is fragile in case of conflict.

Manipulating Basis Objects

Some functions that work with bases:

```
plot(bbasis)
```

plots `bbasis`.

```
eval.basis(0:365,fbasis)
```

evaluates `fbasis` at times 0:365.

```
inprod(bbasis,fbasis)
```

produces the inner product matrix $J_{ij} = \int \phi_i(t)\psi_j(t)dt$. Additional arguments allow use of $L\Phi$ for linear differential operators L.

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Functional Data (`fd`) Objects

Stores functional data: a list with elements

- `coefs` array of coefficients
- `basis` basis object
- `fdnames` defines dimension names

```
fdobj = fd(coefs,bbasis)
```

creates a functional data object with coefficients `coefs` and basis `bbasis` `coefs` has three dimensions corresponding to

1. index of the basis function
2. replicate
3. dimension

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Functional Arithmetic

`fd` objects can be manipulated arithmetically

`fdobj1+fdobj2`, `fdobj1^k`, `fdobj1*fdobj2`

are defined pointwise.

`fd` objects can also be subset

`fdobj[3,2]`

gives the 2nd dimension of the 3rd observation

Additionally

`eval.fd(0:365,fdobj)` returns an array of values of `fdobj` on 0:365.

`deriv.fd(fdobj,nderiv)` gives the `nderiv`-th derivative of `fdobj`.

`plot(fdobj)` plots `fdobj`

`eval.fd` and `plot` can also take argument `nderiv`.

Lfd Objects

Define smoothing penalties

$$Lx = D^m x - \sum_{j=0}^{m-1} \alpha_j(t) D^j x$$

and require the α_j to be given as a list of `fd` objects.

Two common shortcuts:

`int2Lfd(k)` creates an `Lfd` object $Lx = D^k x$

`vec2Lfd(a)` for vector `a` of length `m` creates an `Lfd` object $Lx = D^m x - \sum_{j=1}^m a_j D^{j-1} x$.

In particular

```
vec2Lfd(c(0,-2*pi/365,0))
```

creates a Harmonic acceleration penalty $Lx = D^3 x + \frac{2\pi}{365} D x$.

fdPar Objects

This is a utility for imposing smoothing. It collects

- `fdobj` an `fd` (or a `basis`) object.
- `Lfdobj` a `Lfd` object.
- `lambda` a smoothing parameter.

bifd Objects

Represents functions of two dimensions s and t as

$$x(s,t) = \sum_{i=1}^{K_1} \sum_{j=1}^{K_2} \phi_i(s)\psi_j(t)c_{ij}$$

requires

- `coefs` for the matrix of c_{ij}.
- `sbasis` basis object defining the $\phi_i(s)$.
- `tbasis` basis object defining the $\psi_j(t)$.

Can also be evaluated (but not plotted).

`bifdPar` objects store `bifd` plus `Lfd` objects and λ for each of s and t.

Smoothing Functions

Main smoothing function is `smooth.basis`

```
data(daily)
argvals = (1:365)-0.5
fdParobj = fdPar(fbasis,int2Lfd(2),1e-2)
tempSmooth =
smooth.basis(argvals,daily$tempav,fdParobj)
```

smooths the Canadian temperature data with a second derivative penalty, $\lambda = 0.01$. Along with an `fd` object it returns

`df`	equivalent degrees of freedom
`SSE`	total sum of squared errors
`gcv`	vector giving GCV for each smooth

Typically, λ is chosen to minimize average `gcv`.

Note: numerous other smoothing functions, `Data2fd` just returns the `fd` and can avoid the `fdPar` object, `data2fd` is depricated.

Functional Statistics

Basic utilities:

`mean.fd`	mean `fd` object
`var.fd`	Variance or covariance (`bifd` object)
`cor.fd`	Correlation (given as a matrix)
`sd.fd`	Standard deviation (root diagonal of `var.fd`)

In addition, fPCA obtained through

```
temppca=pca.fd(tempfd$fd,nharm=4,fdParobj)
```

(Smoothing not strictly necessary). `pca.fd` output:

`harmonics`	`fd` objects giving eigen-functions
`values`	eigen values
`scores`	PCA scores
`varprop`	Proportion of variance explained

Diagnostics plots given by `plot(temppca)`

Resources

- Ramsay and Silverman, 2005, "Functional Data Analysis", Springer
- Ramsay and Silverman, 2002, "Applied Functional Data Analysis", Springer
- Ramsay, Hooker and Graves, 2009, "Functional Data Analysis in R and Matlab", Springer
- **www.functionaldata.org**
- `fda` packages for both `R` and Matlab.
- In `R` package: code available to produce examples from all three books.

Questions?

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