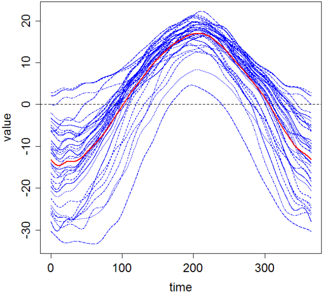
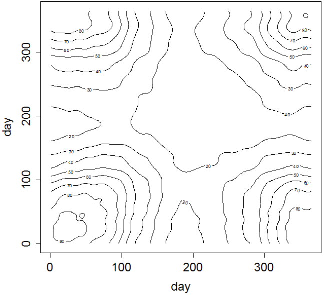
Understanding the Distribution of Collections of Functions

Summary statistics:

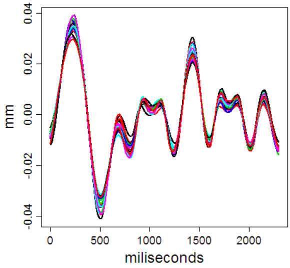
- mean $\bar{x}(t) = \frac{1}{n}\sum x_i(t)$
- covariance $\sigma(s,t) = \frac{1}{n}\sum (x_i(s) - \bar{x}(s))(x_i(t) - \bar{x}(t))$

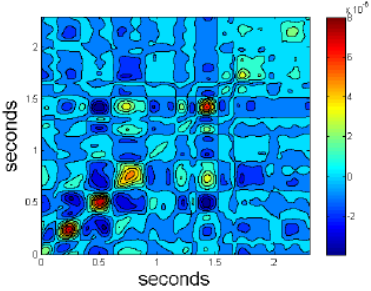




Exploring Functional Covariance

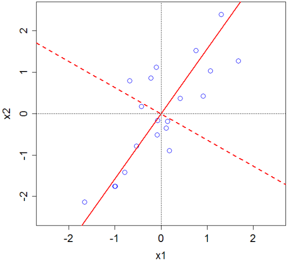
Covariance surfaces provide insight but do not describe the major directions of variation.



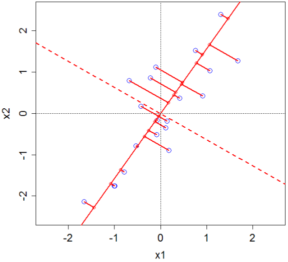


Multivariate Principal Components Analysis

- Directions of greatest variation



- Dimension reduction – subspace closest to the data



Frequently picks out interpretable contrasts.

A Little Analysis

- If $\mathbf{x}$ has covariance Σ, the variance of $u^T\mathbf{x}$ is $u^T\Sigma u$.
- To maximize $u^T\Sigma u$ with $u^T u = 1$ we solve the eigen-equation

$$\Sigma u = \lambda u$$

Mechanics of PCA

- Estimate covariance matrix: $\Sigma = \sum(\mathbf{x}_i - \bar{\mathbf{x}})(\mathbf{x}_i - \bar{\mathbf{x}})^T$
- Take the eigen-decomposition of $\Sigma = U^T D U$
- Columns of U are orthogonal; represent a new basis
- D is diagonal; entries give variances of data along corresponding directions U.
- $d_k / \sum d_k$ = "proportion of variance explained".
- Order D, U in terms of decreasing d_i.
- u_k is the k-th column of U. It is the k-th principal component.
- From original data, $\mathbf{x}_i$, $(\mathbf{x}_i - \bar{\mathbf{x}})^T u_k$ is the k-th principal component score; co-ordinate in new basis.

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- $X_i(t)$ is projected to $s_{i1}, \ldots, s_{iK}$: $X_i(t) = \sum_{k=1}^{K} s_{ik} w_k(t)$

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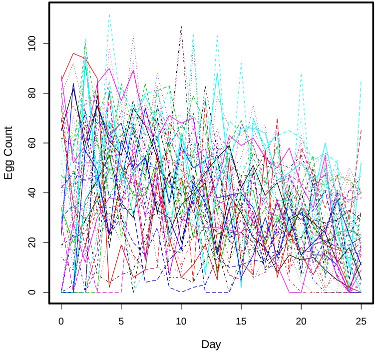
- Top functional principal components (FPC) are represented by a set of flexible basis functions such as B-spline basis.
- Shapes of top FPCs are simple.

One example

- Number of eggs laid by 50 Mediterranean fruit flies over 25 days
- Objective: Exploring major modes of variability in 50 curves



Introduction of FPCA

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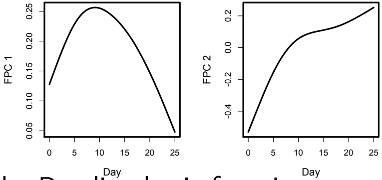
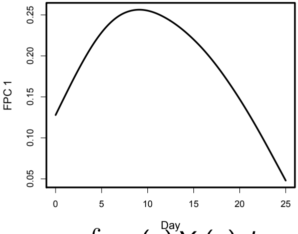
Top Two FPCs of the medfly data



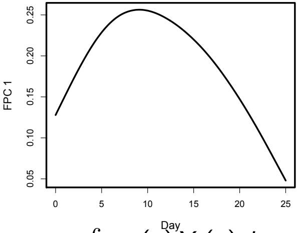
- Represented by B-spline basis functions;
- Explain 91.6% of total variations of data;
- Simple trends.

Interpretation of First FPC



- First FPC score: $s_{i1} = \int w_1(t) X_i(t) dt$
- First FPC: Explains around 62.2% of total variability.
- First FPC: Positive over the whole time interval.

Interpretation of First FPC



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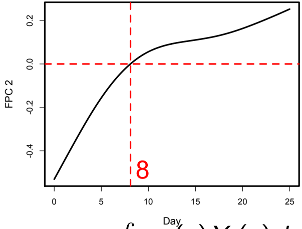
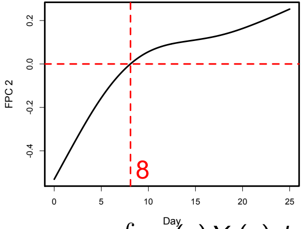
- Interpretation of First FPC score: Weighted average of the number of eggs laid by 50 Mediterranean fruit flies over 25 days.

Interpretation of Second FPC



- Second FPC score: $s_{i1} = \int w_1(t) X_i(t) dt$
- Second FPC: Explains around 29.4% of total variability.
- Second FPC: Positive over the whole time interval.

Interpretation of Second FPC



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- Interpretation of Second FPC score: Change of the number of eggs laid by 50 Mediterranean fruit flies after 8 days.

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- $d_j = \mathrm{Var}(s_{ij})$ for given j
- d_j represents amount of variation in the direction $w_j(t)$.
- $\frac{d_j}{\sum_{j=1}^{\infty} d_j}$ is the proportion of variance explained.

Computing FPCA

Components solve the eigen-equation

$$\int \sigma(s,t) w_i(t) dt = \lambda w_i(t)$$

Option 1

1. take a fine grid $\mathbf{t} = [t_1, \ldots, t_K]$
2. find the eigen-decomposition of $\Sigma(\mathbf{t}, \mathbf{t})$
3. interpolate the eigenvectors

Option 2 (in `fda` library)

1. if the $x_i(t)$ have a common basis expansion, so must the eigen-functions
2. can re-express eigen-equation in terms of co-efficients

Backstage Linear Algebra

- Centered curves $\mathbf{x}(t) = \mathbf{C}\phi(t)$
- $\sigma(s,t) = n^{-1}\phi^T(s)\mathbf{C}^T\mathbf{C}\phi(t)$
- $w(t) = \phi^T(t)\mathbf{b}$
- Want to maximize

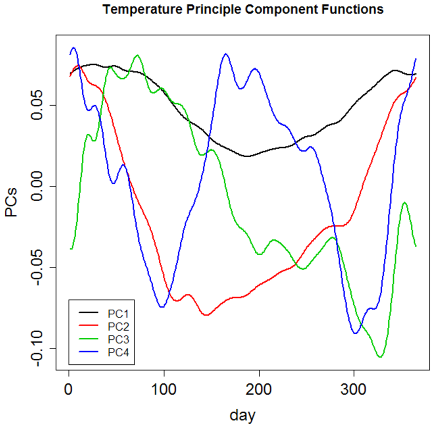
$$\int \sigma(s,t)w(t)dt = \rho w(s)$$

subject to

$$\int [w(t)]^2 dt = \mathbf{b}^T \int \phi(t)^T \phi(t) dt \mathbf{b} = 1$$

- $\mathbf{W} = \int \phi(t)\phi^T(t)dt$
- Substitute $\mathbf{u} = \mathbf{W}^{1/2}\mathbf{b}$ and take the PCA of $\mathbf{W}^{1/2}\mathbf{C}^T\mathbf{C}\mathbf{W}^{1/2}$

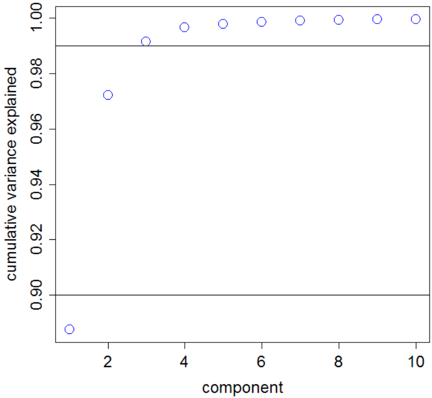
Canadian Temperature Data



- PC1 – over-all temperature
- PC2 – relative temperature of winter and summer
- PC3 – contrast between fall and spring
- PC4 – relative lengths of summer/winter

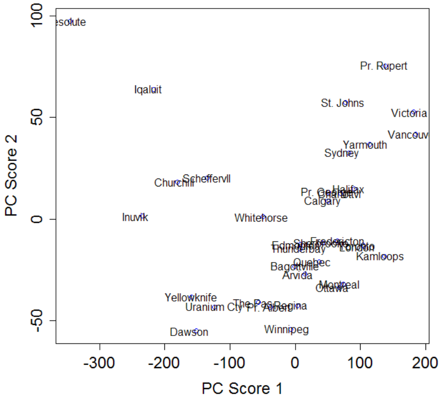
Canadian Temperature Data

We can alternatively calculate how many components are needed to capture 90% of the total variation in the data.



Canadian Temperature Data

Sanity check: we can plot the first two PC scores for each observation.

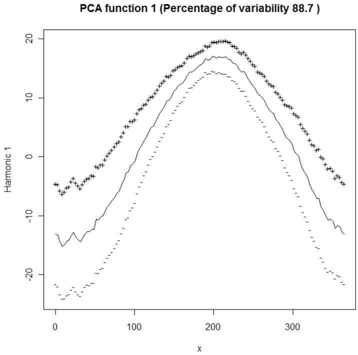


- First PC: over-all temperature.
- Second PC: contrast between Summer and Winter.

Display of Principal Components

Best way to obtain an idea of variation for each component is to plot

$$\bar{x}(t) \pm 2\sqrt{d_i}w_i(t)$$



Summary

- PCA = means of summarizing high dimensional covariation
- fPCA = extension to infinite-dimensional covariation
- Representation in terms of basis functions for fast(er) computation