Dimension reduction for high dimensional regression problems based on local principal curves

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joint work with
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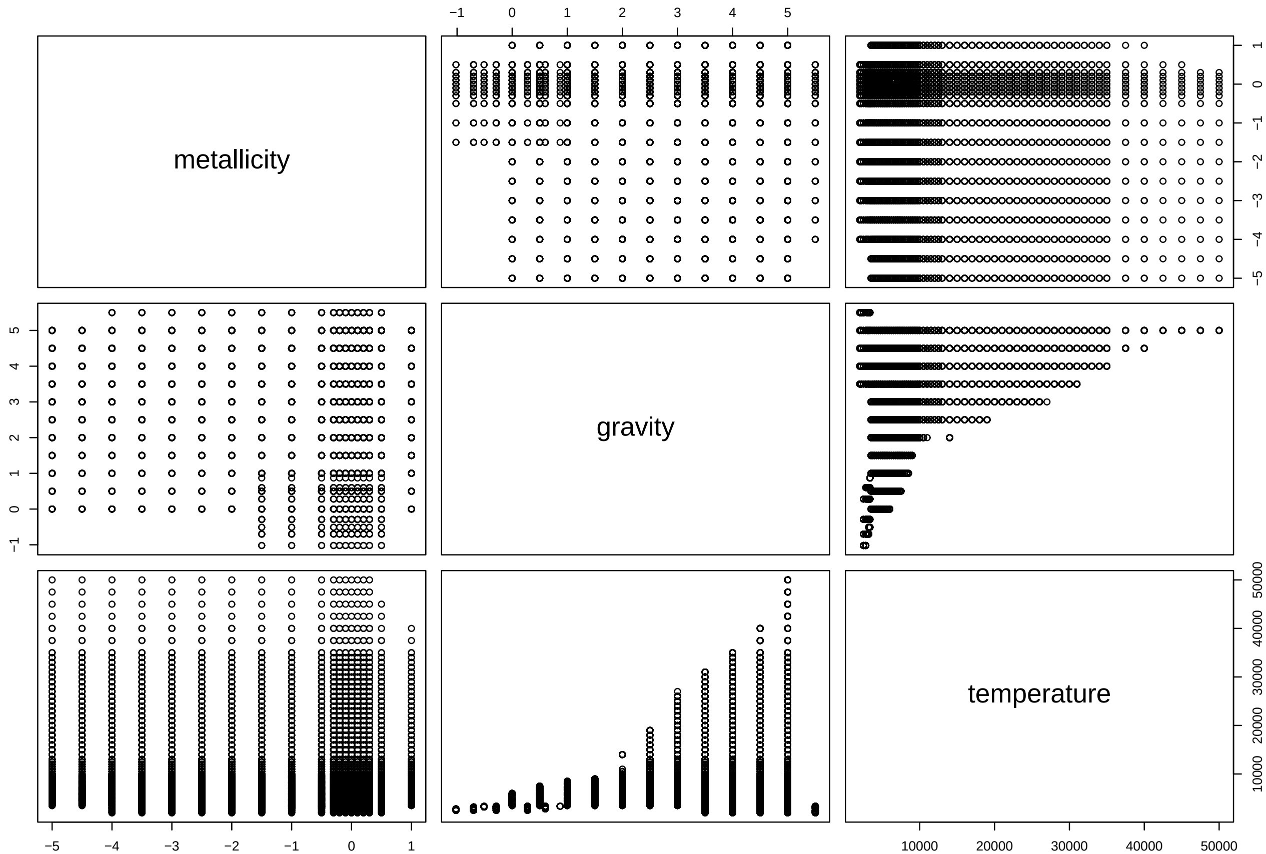
in collaboration with Gerhard Tutz (LMU Munich) and Coryn Bailer-Jones (MPIA Heidelberg).

Motivation: G I data

- GAIA is an astrophysics mission of the European Space Agency (ESA) which will undertake a detailed survey of over 10^9 stars in our Galaxy and extragalactic objects.
- Satellite to be launched in 2011.
- Aims of the mission (among others)
  - Classify objects (star, galaxy, quasar,...)
  - Determine astrophysical parameters ("APs": temperature, metallicity, gravity) from spectroscopic data (photon counts at certain wavelengths).
- Work on these aims is led by the group "Astrophysical parameters" based at MPIA Heidelberg, being part of the DPAC (Data Processing and Analysis Consortium) which is responsible for the general handling of data from the GAIA mission.
- Yet, one has to work with simulated data generated through complex computer models.

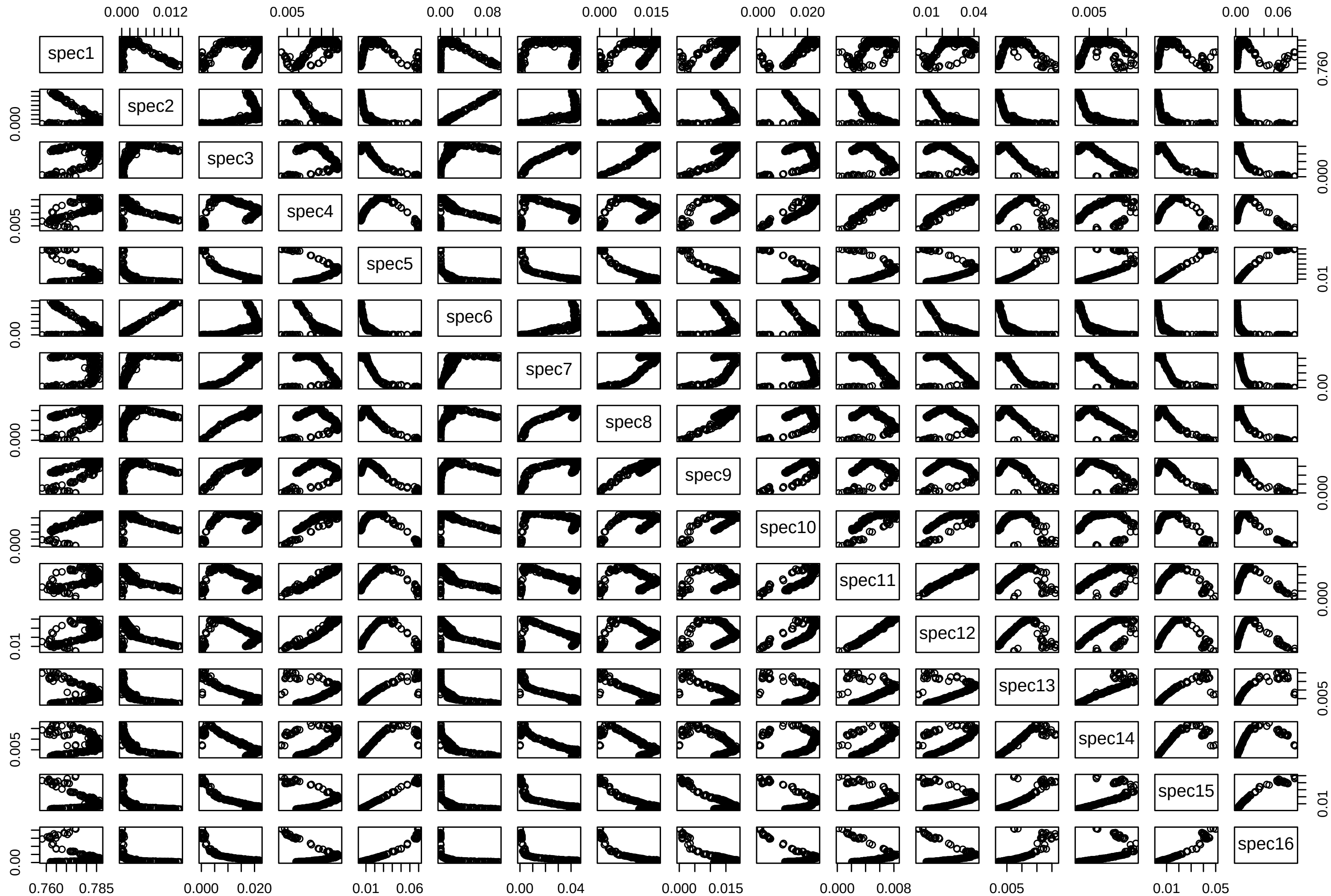
Simulated G I data

- Photon counts are simulated from APs
- AP Design space:



Simulated G I data (cont.)

- Photon counts simulated from APs through computer models:



G I data: Estimation of Ps

- Note that, for the actual estimation problem, the photon counts form the *predictor space* and the AP's form the *response space* (this is opposite to the direction of simulation!)
- As a consequence, the regression problem may be degenerate (i.e., one set of photon counts may be associated to two different APs). We focus here on the temperature, which features the least amount of degeneration.
- Can one use a linear model here?
  - For instance, temperature as response:

```
> gaia.lm <- lm(temperature˜ spec1 + spec2 +
                ...+ spec16, data= gaia)
```

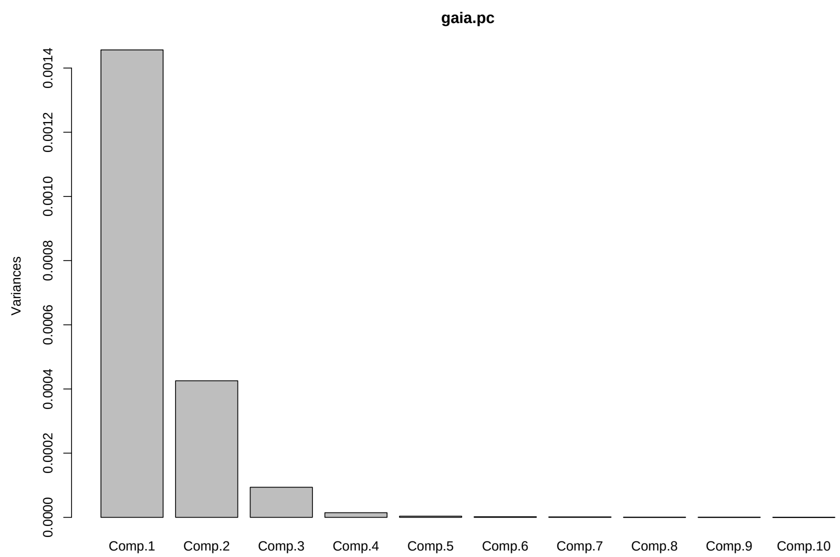
G l data: Estimation of Ps (cont.)

```
> summary(gaia.lm)
Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept) -14033286   21104764  -0.665    0.506
spec1        14065842   21104812   0.666    0.505
spec2        14216977   21107526   0.674    0.501
spec3        13982281   21106961   0.662    0.508
spec4        13987405   21109664   0.663    0.508
.     .         .        .        .
.     .           .        .        .
spec16       13886697   21106076   0.658    0.511

Residual standard error: 1978 on 983 degrees of freed
```

All variables are insignificant.

Dimension reduction

- Usual remedies:
  - Model/ variable selection procedures
  - Dimension reduction techniques
- The second one is obviously the more promising here.
- Look at scree plot:



- Two (or maximal three) components appear to be sufficient.

Principal component regression

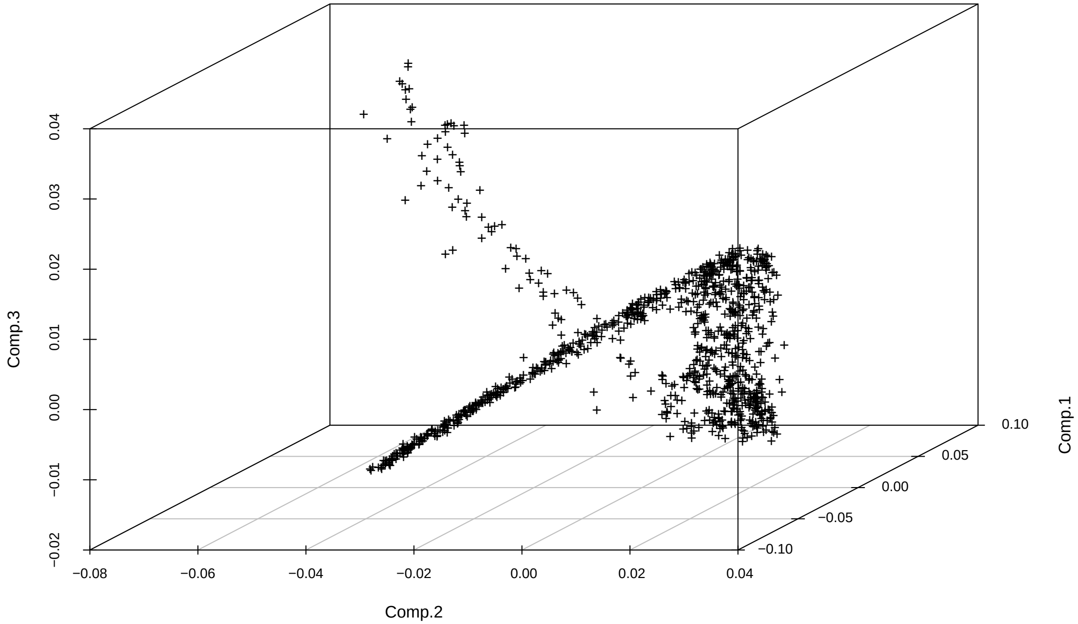
- Fit temperature against the first three PC scores:

```
gaia.pclm  <- lm(temperature ~ Comp1 + Comp2 +
               + Comp3, data = gaiapc)

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept)   10835.90      65.14  166.34   <2e-16 **
Comp1       -187339.39    1706.85 -109.76   <2e-16 **
Comp2       -173967.35    3157.61  -55.09   <2e-16 **
Comp3       -155314.86    6726.19  -23.09   <2e-16 **

Residual standard error: 2060 on 996 degrees of freed
```

- This is somewhat more appropriate than the full linear model, but....

Principal component scores

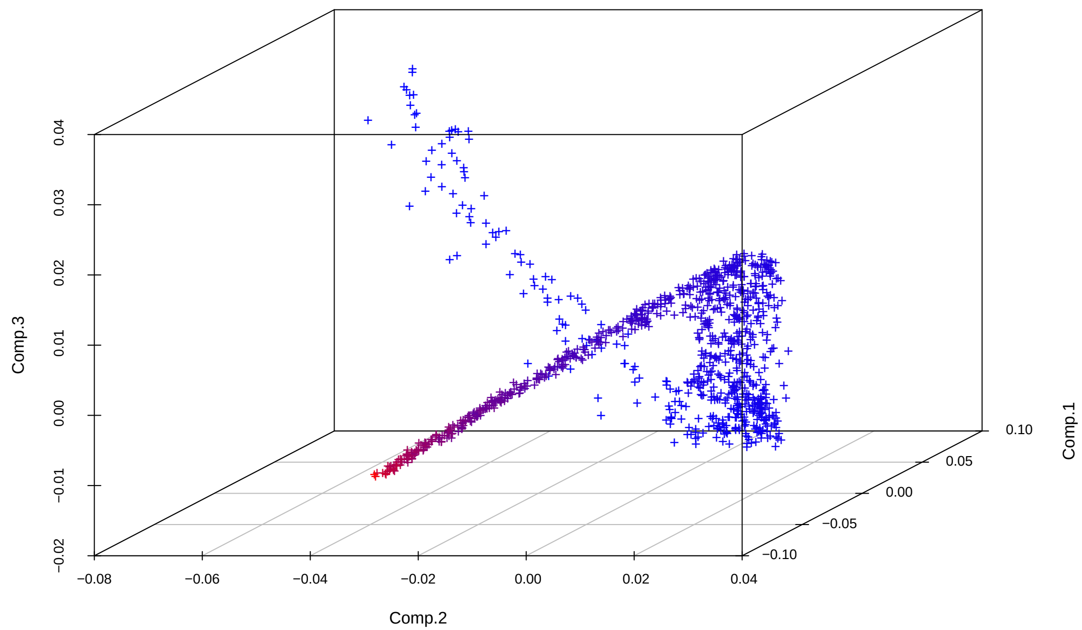
- We plot the the first three principal component scores



- Actually, we seem to need only *one* parameter if we were able to lay a smooth curve through the data cloud.

Principal component scores

- We plot the the first three principal component scores and shade higher temperatures red.



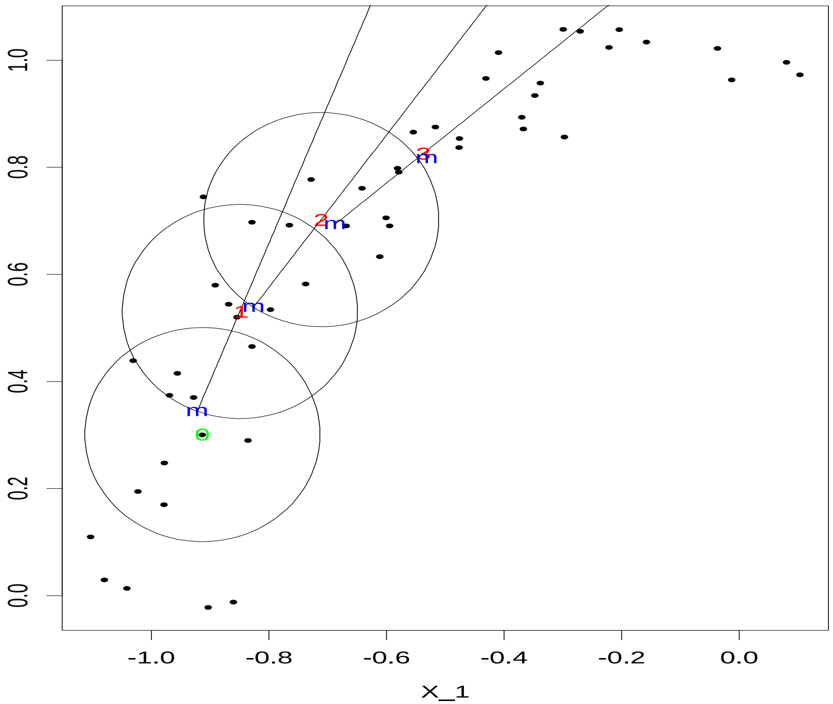
- Actually, we seem to need only *one* parameter if we were able to lay a smooth curve through the data cloud.
- The parameterization along such a curve would be informative w.r.t. to the target variable, temperature.

G I data and principal curves

- Hence, the following is to do:
  (1) Estimate the smooth curve capturing the structure of the (three-dim!) predictor space.
  (2) Parameterize this curve and project all data points onto it.
  (3) Fit temperature (or other APs) against the (1-dim.) projections.
- Step (1) is a task for principal curves. There are a couple of principal curve algorithms available, but not all of them are suitable for task (2).
- We concentrate here on local principal curves.

Local principal curves (LPCs)

- Einbeck, Tutz & Evers (2005)
- Idea: Calculate alternately a local center of mass and a first local principal component.



0: starting point,
m: points of the LPC,
$1, 2, 3$: enumeration of steps.

lgorithm for LPCs

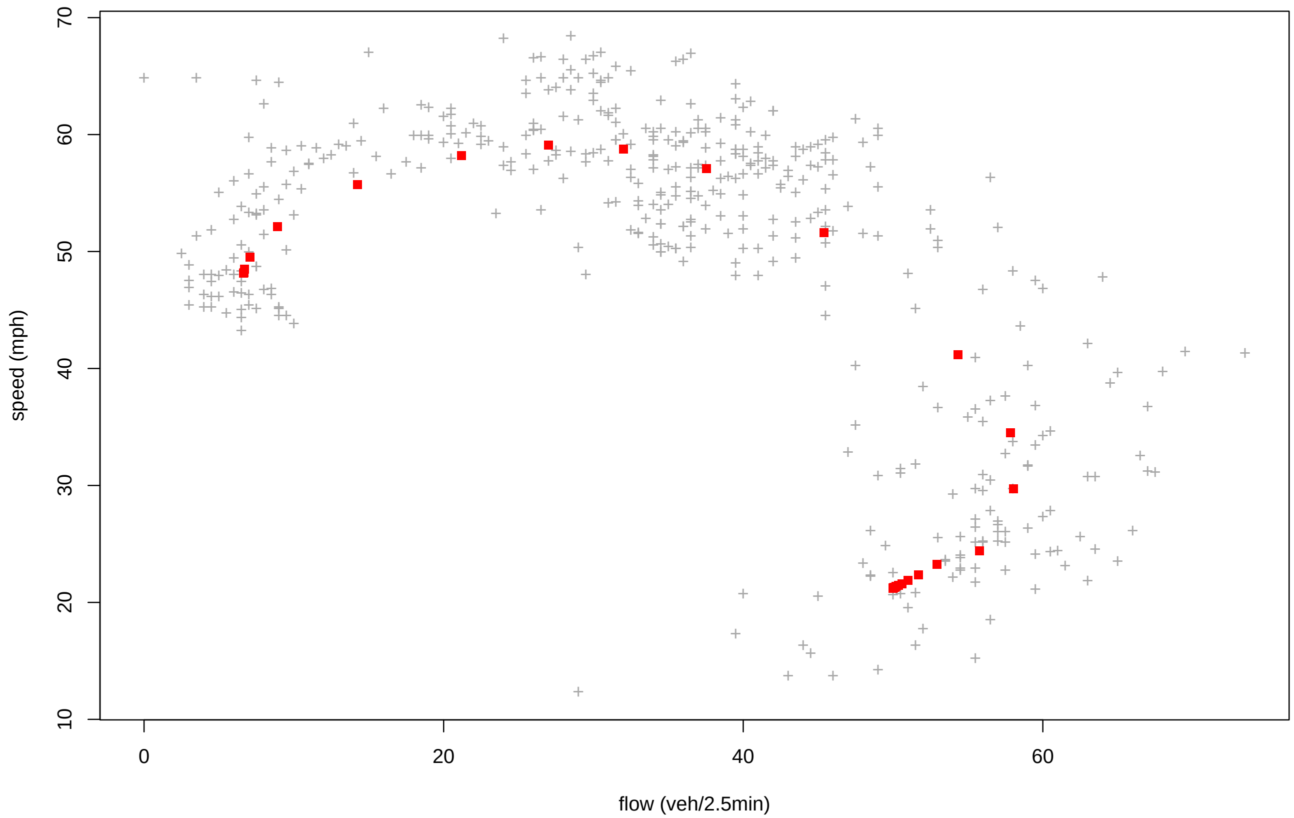
Given: A data cloud $X = (X_1, \ldots, X_n)$, where $X_i = (X_{i1}, \ldots, X_{id})$.

1. *Choose a starting point x_0. Set $x = x_0$.*
2. *At x, calculate the local center of mass $\mu^x = \sum_{i=1}^n w_i X_i$, where $w_i = K_H(X_i - x)X_i / \sum_{i=1}^n K_H(X_i - x)$, with bandwidth matrix H.*
3. *Compute the 1^{st} local eigenvector γ^x of $\Sigma^x = (\sigma_{jk}^x)_{(1 \leq j,k \leq d)}$, where*
$$\sigma_{jk}^x = \sum_{i=1}^n w_i (X_{ij} - \mu_j^x)(X_{ik} - \mu_k^x).$$
4. *Step from μ^x to $x := \mu^x + t_0 \gamma_1^x$.*
5. *Repeat steps 2. to 4. until the μ^x remain constant. Then set $x = x_0$, set $\gamma^x := -\gamma^x$ and continue with 4.*

The sequence of the local centers of mass μ^x makes up the local principal curve (LPC).

Simpler example: Speed-flow data

- Data recorded on the Californian Freeway FR57-N on 9th of July 2007:

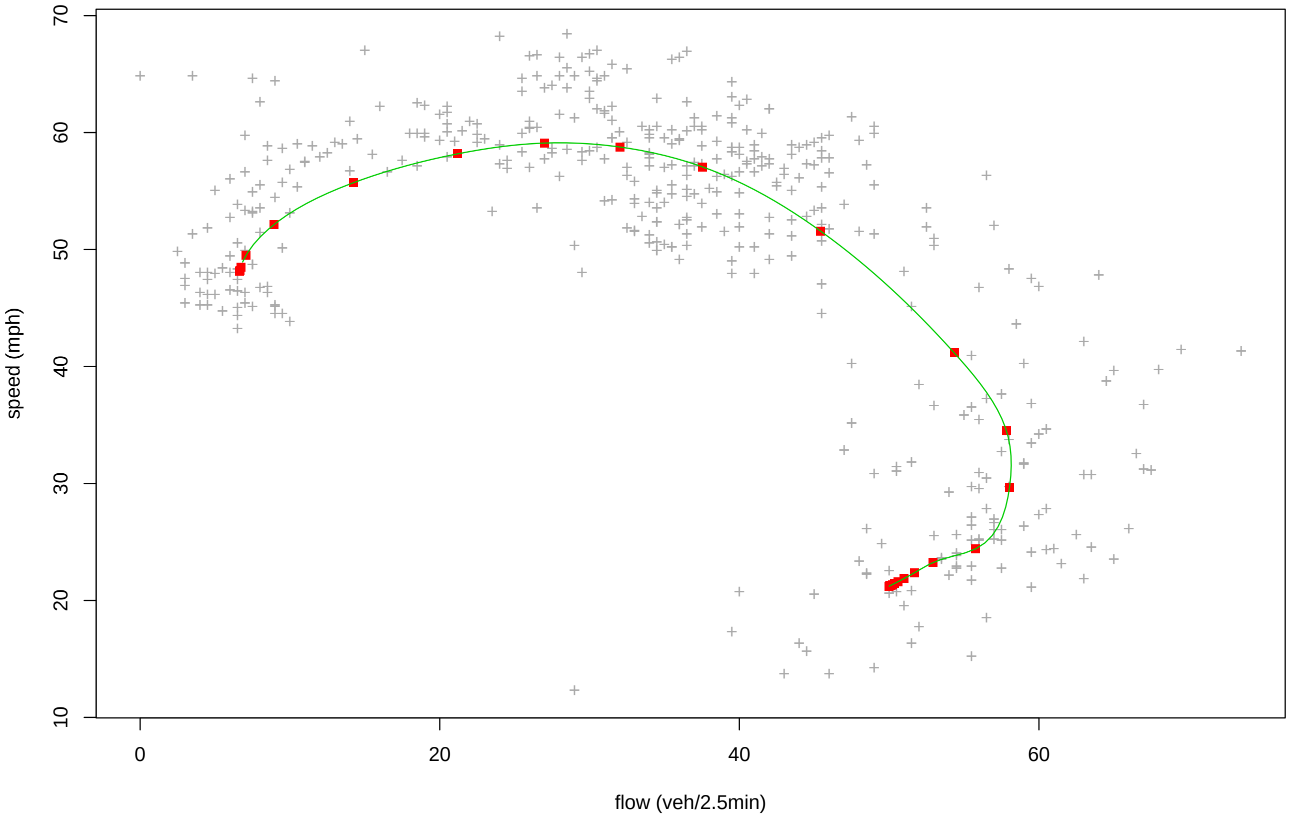


(data from: PemS)

- The red squares correspond to the points μ^x making up the LPC.

Example: Speed-flow data

- Technical question: How to connect the points?
- For descriptive purposes, a linear interpolation is sufficient.
- If one wants to compute projections onto it, a cubic spline can be laid through the curve:



Parametrization

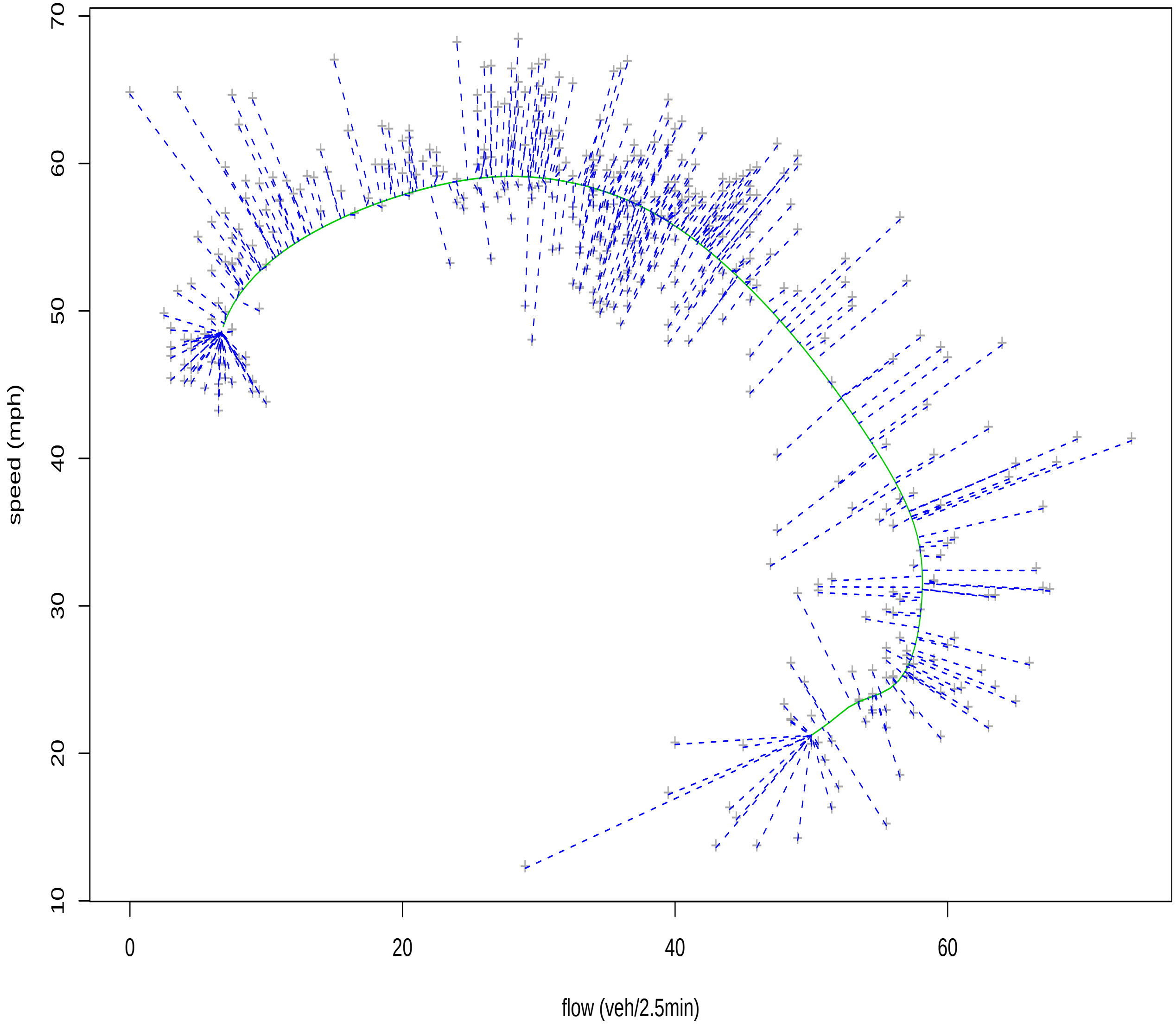
- Next, the origin is fixed to $t = 0$ at one of the two ends. We consider the LPC as a curve

$$f : \mathbb{R} \longrightarrow \mathbb{R}^2,\, t \mapsto \left(\begin{array}{c} x(t) \\ y(t) \end{array} \right)$$

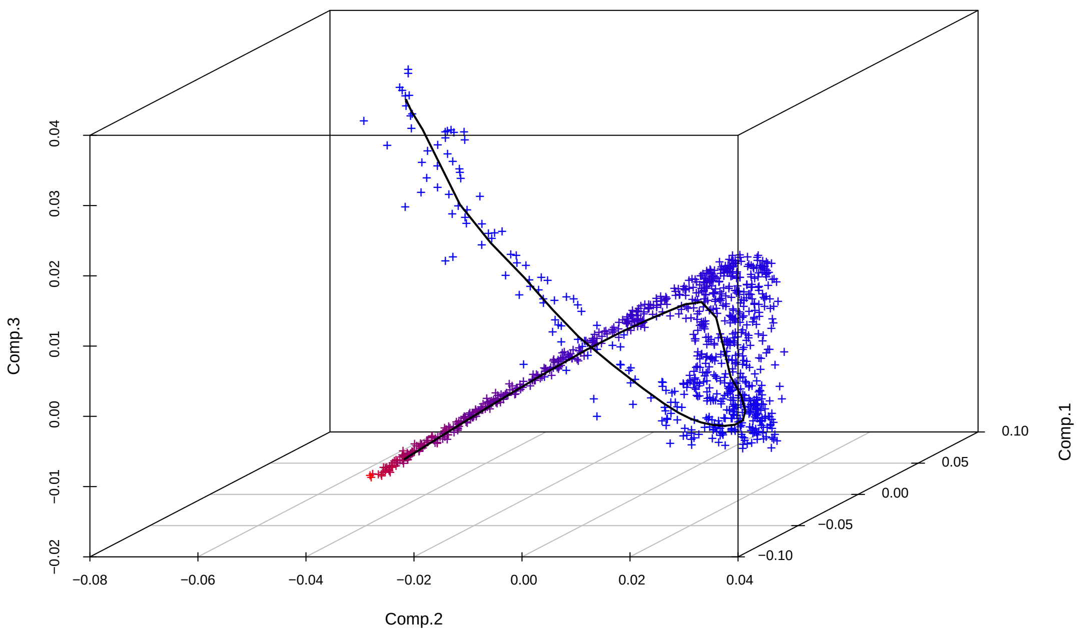
  and the parameterization along the curve is defined through the arc length w.r.t this origin.

- Each point (x_i, y_i) can then be projected on the point of the curve nearest to it, yielding the corresponding projection index t_i, which could, for example, be used as one-dimensional representant in a regression problem involving speed and flow as covariates.

Projections



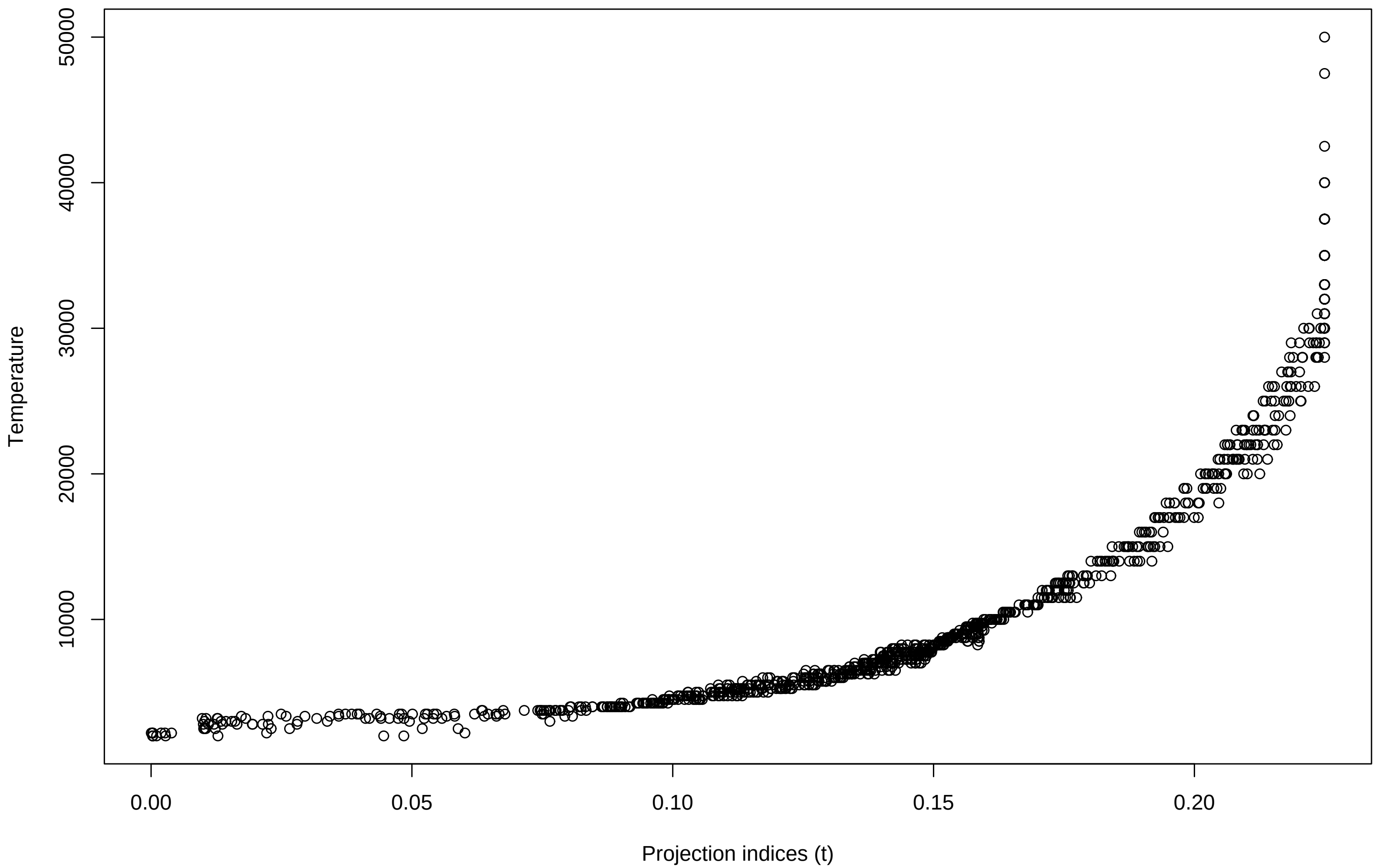
LPCs through G I data



- Local principal curves seem to capture the structure of the data cloud adequately.
- If this curve is to be used for regression, then:
  - Fit the spline through the 3-dim LPC points
  - Compute projection indices t_i of all data points onto this spline

LPC Regression with G I data

- Assume we want to predict stellar temperature from spectral data.
- This is now a simple one-dimensional regression problem $y_i = f(t_i) + \varepsilon_i$:



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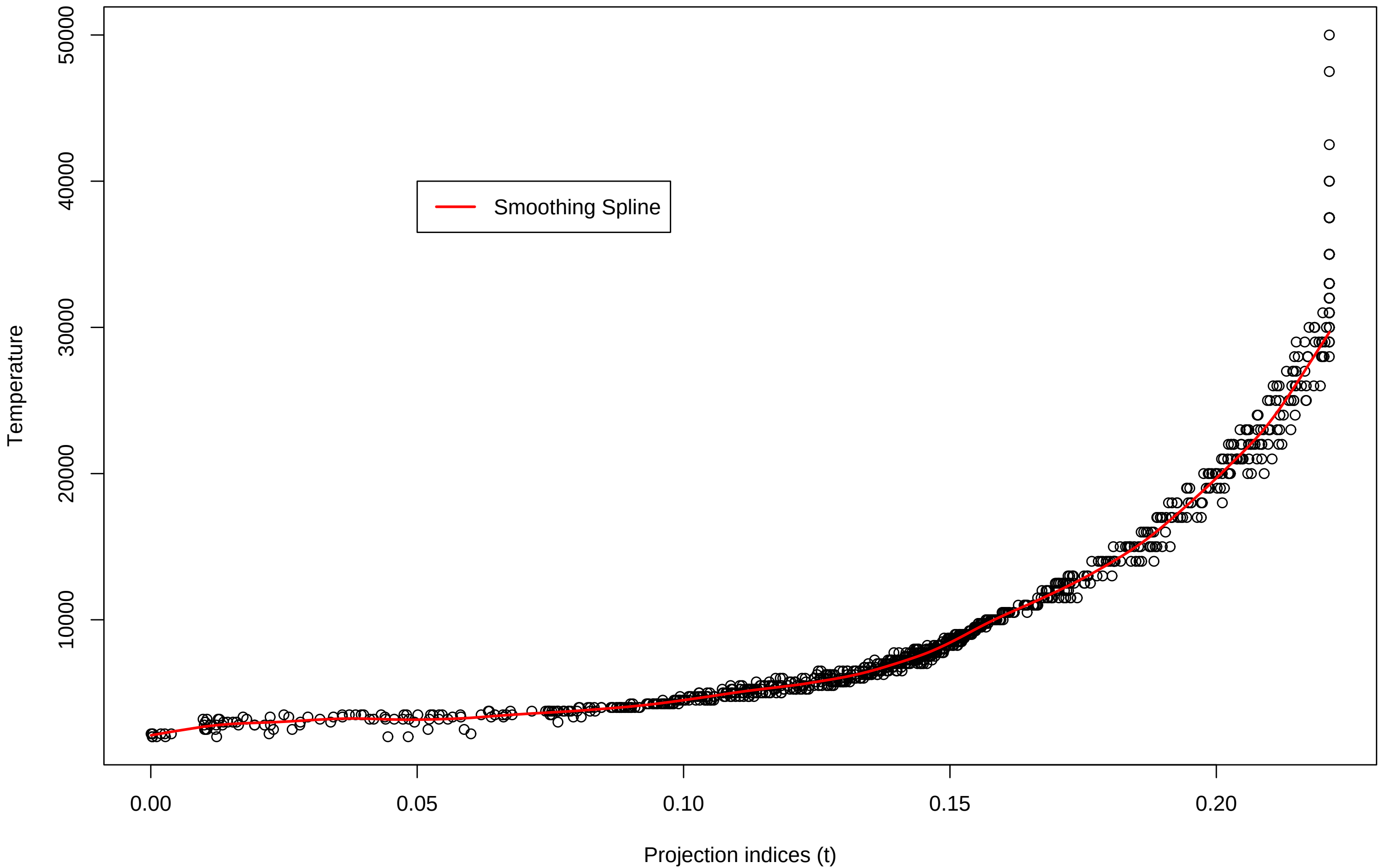
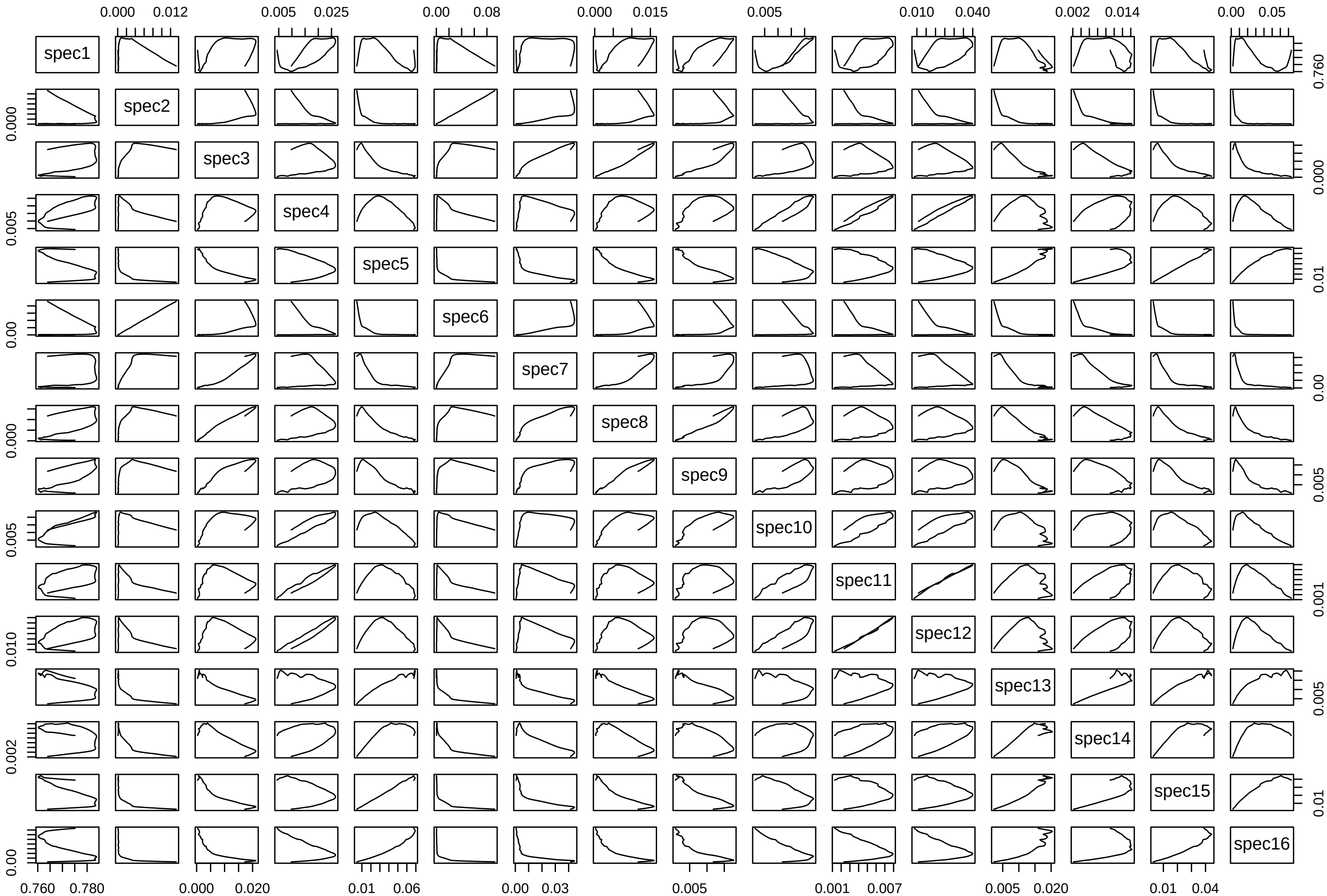


Is there a shortcut?

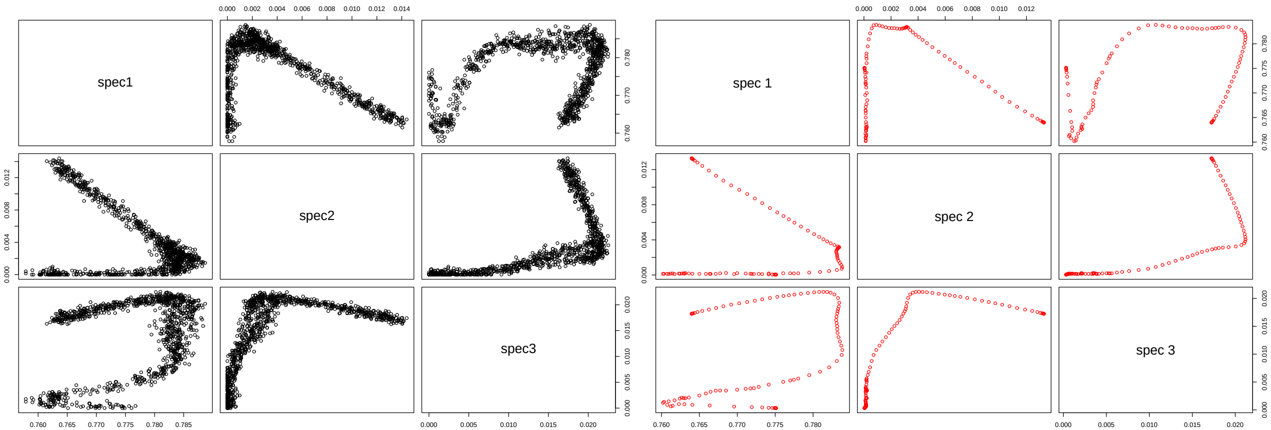
- LPC fitted *directly* through 16- dimensional space:



Direct data compression with LPCs

- Zoom into the the first three dimensions:

Data LPC



- Approximating the data cloud directly by a LPC works in principle, but is potentially "dangerous": As data gets sparse in high dimensions, the LPC may miss important patterns of the predictor space and its performance will depend on the choice of the starting point.

Prediction

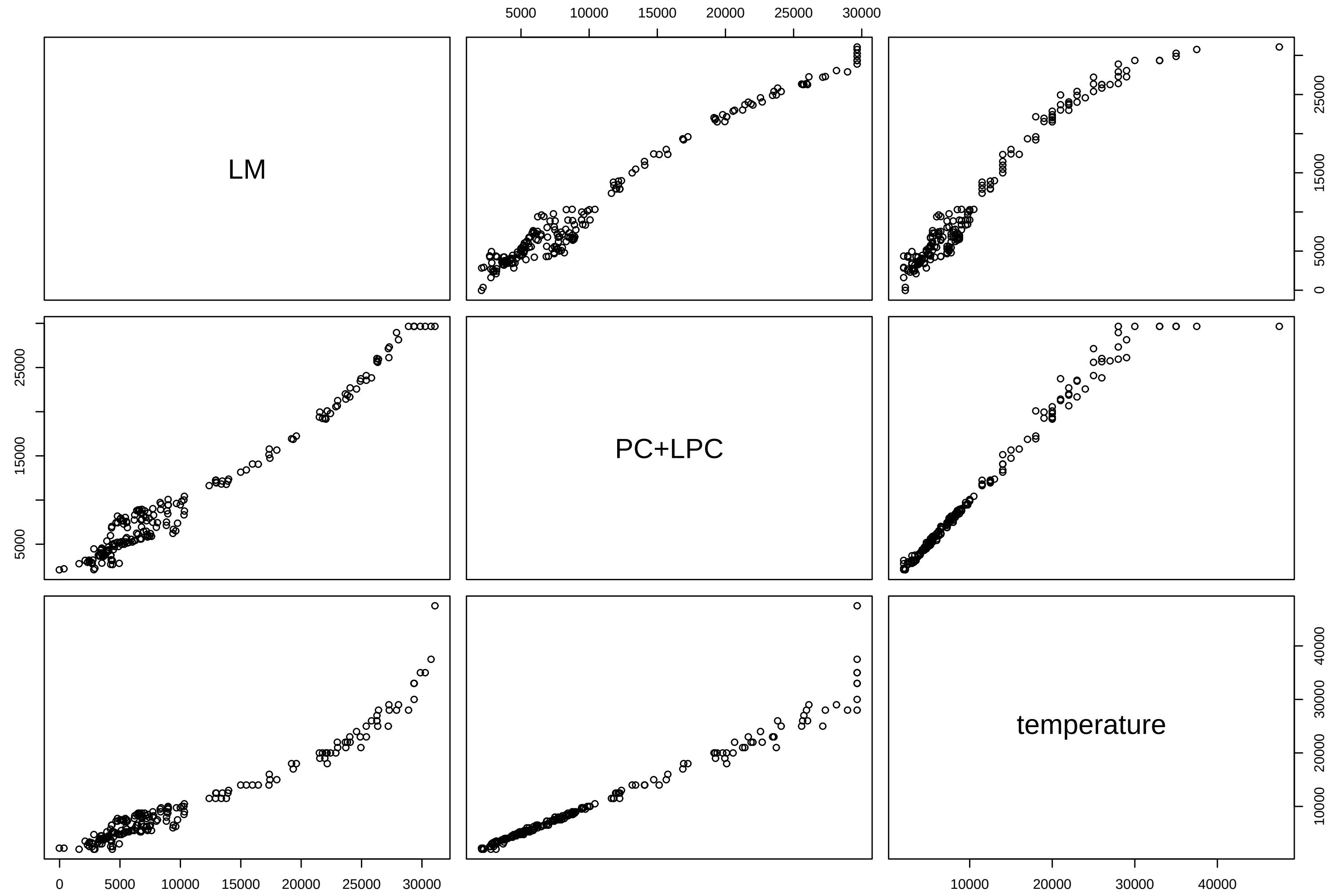
- For a new observation x_{new} (i.e., here, a new set of spectra), prediction proceeds as follows:
  - Project x_{new} onto the LPC, giving t_{new}.
  - Compute $\hat{y}_{new} = f(t_{new})$ from the fitted regression model.
- Comparison: Prediction error ($*10^3$) for 200 observations sampled from the training data set:

	LM	PC+Regr	LPC+Regr	PC+LPC+Regr
average($\hat{\varepsilon}_i^2$)	4,119	4,395	2,215	2,633
median($\hat{\varepsilon}_i^2$)	1,035	1,300	66	51

where $\hat{\varepsilon}_i$ is the difference between true and predicted temperature.

Take care with boundaries!

- Compare predicted values through LM and PC+LPC with true temperature values:



Robustness issues

- LPCs are by construction resistant to outlying data patterns, if the starting point is fixed.
- However, resistance is not necessarily a desired feature when exploring the *covariate space*. Here, it is important that *all* regions of it are covered, even if outlying.
- If the data pattern is not connected but scattered in space, one needs multiple/ branched/ disconnected LPCs to describe it.
    - Technically possible (Einbeck, Tutz, Evers, 2005b), but yet to incorporate into regression framework.....
- An important issue is robustness to the choice of the starting point, which is the more critical the more sparse the data are.

Conclusion and Outlook

- Local principal curves are well suited to compress complex high-dimensional data structures, as long as the intrinsic dimensionality of the data cloud is close to one.
- When the intrinsic dimensionality is two or larger, the extension to *local principal manifolds* should be considered.

Conclusion and Outlook

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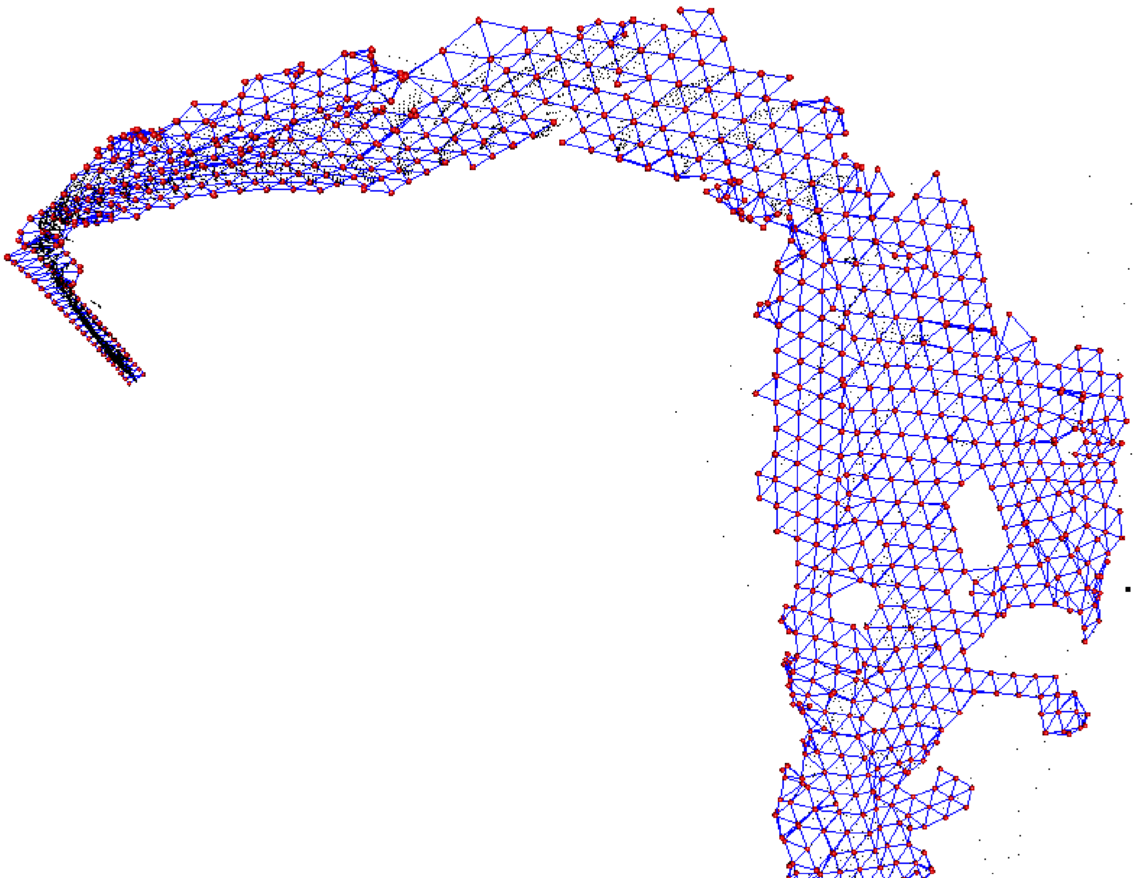

...work in progress!

Literature

Einbeck, Tutz & Evers (2005): Local principal curves. *Statistics and Computing* **15**, 301–313.

Einbeck, Tutz & Evers (2005b): Exploring multivariate data structures with local principal curves. In: Weihs, C. and Gaul, W. (Eds.): *Classification - The Ubiquitous Challenge*. Springer, Heidelberg.

Einbeck, Evers & Bailer-Jones (2007): Representing complex data using localized principal components with application to astronomical data. In: Gorban, Kegl, Wunsch, & Zinovyev: Principal Manifolds for Data Visualization and Dimension Reduction; *Lecture Notes in Computational Science and Engineering* **58**, 180–204.