Semi-Parametric Manifold Clustering

Estimating Polynomial Curves

Problem Setup

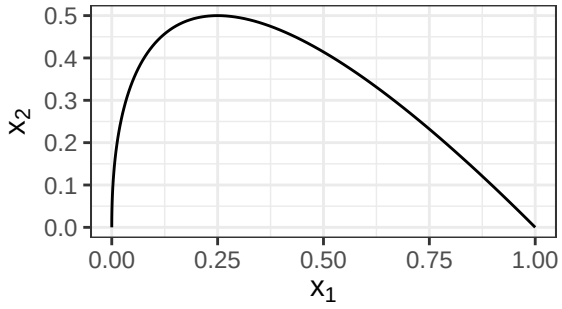
Let:

- $T_1, ..., T_n \overset{\text{iid}}{\sim} F$ with support $[0, 1]$.
- $g(\cdot, \theta) : [0, 1] \mapsto \mathcal{X} \subset \mathbb{R}^d$.
- $X_1, ..., X_n = g(T_1), ..., g(T_n)$

Assuming some parametric form of g with parameters θ, we want to find $\hat{\theta}$, some "reasonable" estimate for θ. We observe X_i but not T_i.

For now, we limit $d = 2$ and g to quadratic functions.

Example 1. *Let $g(t) = (t^2, 2t(1-t)) = (0 + 0t + t^2, 0 + 2t - 2t^2)$. (This is the first two dimensions of the Hardy-Weinberg curve). Then $\theta = (0, 0, 1, 0, 2, -2)$.*



If we observe the T_i's, then we can use a standard polynomial regression method to obtain $\hat{\theta}$. Since we do not observe them, the proposed iterative method is as follows:

1. Initialize $\hat{\theta}^{(0)}$ (e.g., randomly).
2. Estimate each $\hat{t}_i^{(s)}$ by minimizing $L(t_i, \hat{\theta}^{(s)}|x_i) = L_i = \|x_i - g(t_i|\hat{\theta}^{(s)})\|^2$.
3. Compute each $\hat{x}_i^{(s)} = g(\hat{t}_i^{(s)}|\hat{\theta}^{(s)})$
4. Estimate $\hat{\theta}^{(s+1)}$ by minimizing $L(\{\hat{t}_i^{(s)}\}, \theta|X) = \sum_i \|x_i - g(\hat{t}_i^{(s)}|\theta)\|^2$.
5. Repeat steps 2-4 until convergence.

If we restrict g to be polynomials, then steps (2) and (4) have closed-form solutions. Alternatively, we can estimate g using more general forms, e.g., splines, which may require approximation.

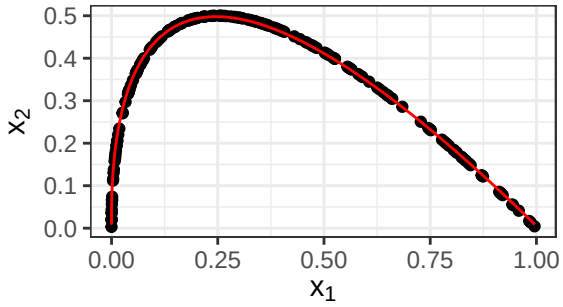
Example 2. *Write $g(t|\theta) = (g_1(t|\theta_1), ..., g_d(t|\theta_d))$ where $g_r(t|\theta_r)$ is the component of g in the r^{th} dimension and θ_r is the vector of parameters for the r^{th} dimension. If g_r are polynomials of degree p, then each θ_r contains up to $p + 1$ entries.*

Given the observed points $x_1, ..., x_n \in \mathbb{R}^d$ and their corresponding index points $t_1, ..., t_n \in \mathbb{R}$, we can find each $\hat{\theta}_r$ individually by $\hat{\theta}_r = A^{-1}b$ where $b \in \mathbb{R}^{p+1}$ and $b_k = \sum_i x_i t_i^k$ and $A \in \mathbb{R}^{(p+1)\times(p+1)}$ and

$A_{kl} = \sum_i t^{(k-1)(l-1)}$.

On the other hand, if we have parameters θ but not the index points t_i, we can minimize each t_i individually by finding the roots of a $p+1$ polynomial with coefficients that depend on $x_1, ..., x_n$ and θ.

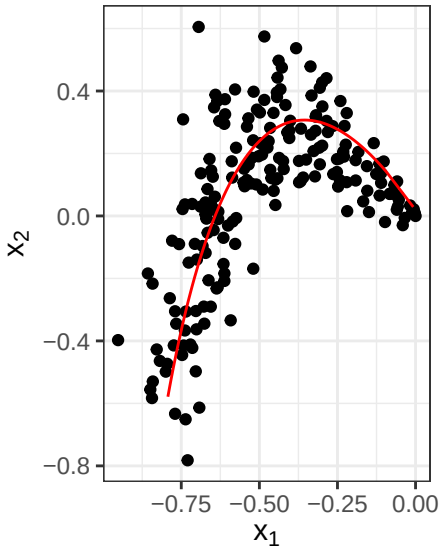
In the following plot, we drew $n = 200$ points from the 2D H-W curve with $T_1, ..., T_n \overset{\text{iid}}{\sim} Uniform(0, 1)$. The red line is the curve that was fit using the above method.



Note: the parameterization of the curve is not unique.

Estimation with Noise

Example 3. *In the next example, we draw $A \sim \text{RDPG}(X)$ using the same H-W curve and sample size as above and estimate the true latent positions (up to rotation).*



A modification to this that is possibly more robust is to use Bezier curves for g. This is the same functional form as the polynomial curves used before, but with orthogonal bases:

$$g(t|p) = \sum_{r=0}^{R} p_r \binom{R}{r} (1-t)^{R-r} t^r$$

where R is the order of the Bezier curve, each p_s is a vector of length d, and, as before, $g : [0, 1] \mapsto \mathbb{R}^d$. Thus, if we fit each p_r, then the procedure is the same as before.

The least squares estimate for $p \in \mathbb{R}^{R \times d}$ is

$$\hat{p} = (T^\top T)^{-1} T^\top X$$

where $T = \begin{bmatrix} t_{\cdot,1} & \cdots & t_{\cdot,R} \end{bmatrix}$ and each $t_{ir} = \binom{R}{r}(1-t_i)^{R-r} t_i^r$, and $X \in \mathbb{R}^{n \times d}$. The same procedure for estimating $t_1, ..., t_n$ can be applied here.

The parameterization for a given curve is not unique. In particular, the above procedure will not necessarily provide $t_1, ..., t_n \in [0, 1]$. One possible remedy for this is to, after estimating the t_i's, normalize them to the unit interval. If we assume $t_1, ..., t_n \overset{\text{iid}}{\sim} Uniform(a, b)$, then the UMVUE are

$$\hat{a} = \frac{n t_{(1)} - t_{(n)}}{n-1}, \hat{b} = \frac{n t_{(n)} - t_{(1)}}{n-1}$$

which yields the normalization transformation $t \leftarrow (t - \hat{a})/(\hat{b} - \hat{a})$.

Alternatively, we can force the t_i's to be approxiately uniform on the unit interval by the transformation $t \leftarrow \hat{F}(t)$, where $\hat{F}$ is the empirical CDF of $t_1, ..., t_n$.

For initialization, we can use a one-dimensional Isomap embedding to estimate the t_i's and use that to estimate $\hat{p}$. Experiments suggest that if the data are well-behaved (i.e., it looks like the curve we are trying to fit), this results in much faster convergence.

Theoretical Framework

If we assume that the points are distributed as $X_i \overset{\text{ind}}{\sim} \mathcal{N}(f(t_i|p), \Sigma(t_i|\phi))$, then we can write the (incomplete) log likelihood as:

$$\ell(p, \phi) = -\frac{1}{2}\sum_i \log|\Sigma(t_i|\phi)| - \frac{1}{2}\sum_i (x_i - f(t_i|p))^\top (\Sigma(t_i|\phi))^{-1}(x_i - f(t_i|p))$$

In the case $\Sigma(t_i|\phi) = \phi I$ and $f(t_i|p) = p^\top \tilde{t}_i$ where $\tilde{t}_i \in \mathbb{R}^{R+1}$ is the Bezier polynomial expansion of order R, then this becomes

$$\ell(p, \phi) = -\frac{nd}{2}\log\phi - \frac{1}{2\phi}\|X - Tp\|_F^2$$

Then given $t_1, ..., t_n$, the MLE of p is again $(T^\top T)^{-1} T^\top X$, and the MLE of ϕ is just $\frac{1}{nd}\|X - T\hat{p}\|_F^2$. And given p, we can estimate each t_i in the same way as before to maximize ℓ (the variance is unnecessary here).

As noted before, the parameterization given by T and p is not unique. We can arbitrarily scale the t_i's and p to obtain the same value of ℓ. Naively performing the proposed algorithm sometimes results in estimates for p that diverge and estimates for t_i's that converge to a single value. To remedy this, we can either scale the t_i's as before, or we can scale p by forcing f to be an arclength parameterization.

Theorem 1. *Let* $x_1, ..., x_n \overset{\text{ind}}{\sim} \mathcal{N}(p^\top \tilde{t}_i, \phi I_d)$*, where each* $x_i \in \mathbb{R}^d$*,* $\tilde{t}_i \in \mathbb{R}^{R+1}$ *such that* $\tilde{t}_{i,r} = \binom{R}{r}(1-t_i)^{R-r}t_i^r$ *for* $i = 1, ..., n$ *and* $r = 0, ..., R$*, and* $p \in \mathbb{R}^{(R+1)\times d}$*.*

Then each iteration of the following decreases the negative log likelihood:

1. $p \leftarrow (T^\top T)^{-1}T^\top X$*, where* $T = \begin{bmatrix}\tilde{t}_1 & \cdots & \tilde{t}_n\end{bmatrix}^\top$ *and* $X = \begin{bmatrix}x_1 & \cdots & x_n\end{bmatrix}^\top$*.*
2. $t_i \leftarrow \arg\min_t \|x_i - p^\top \tilde{t}_i\|^2$*, which can be solved by finding the roots of a polynomial of degree* $2R - 1$*.*

Proof (sketch). For $\Sigma(t_i|\phi) = \phi I$, the negative log likelihood is, up to some additive and multiplicative constants:

$$l(p, \{t_i\}) = \|X - Tp\|_F^2 = X^\top X - 2X^\top Tp + p^\top T^\top Tp$$

To find the minimizer $\hat{p}$ given $t_1, ..., t_n$:

$\nabla_p l = -2T^\top X + 2T^\top Tp = 0 \implies \hat{p} = (T^\top T)^{-1}T^\top X$

To find the minimizer $\hat{t}_i$ given p:

We can rewrite the negative log likelihood as $l(p, \{t_i\}) = \sum_i \|x_i - p^\top \tilde{t}_i\|^2$.

Then each entry of $\nabla_t l$ depends only on t_i, so each t_i can be optimized independently. Furthermore, each $\frac{\partial}{\partial t_i}\|x_i - p^\top \tilde{t}_i\|^2$ is a polynomial in t_i, so it can be minimized by simply finding the roots of the polynomial.

Thus this algorithm is a coordinate descent algorithm, which reduces the objective function with each iteration. □

Theorem 2. *Let* $A^{(n)} \sim \text{RDPG}(F(p, \theta), n)$*, and let* $X^{(n)}$ *be the ASE of* $A^{(n)}$*. Let* $\hat{p}, \{\hat{t}_i\}$ *be the global minimizer of* l *given* $X^{(n)}$*. Then* $l(\hat{p}, \{\hat{t}_i\}) \overset{a.s.}{\to} 0$*.*

Covariance Structures

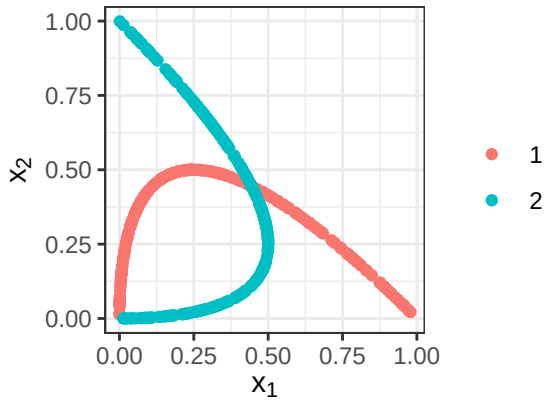
While the CLT property of the ASE allows us to approximate $x_i \sim \mathcal{N}(Wf(t_i|p), W\Sigma(t_i|\phi)W^\top)$, it is unclear what $\Sigma(t_i|\phi)$ looks like, and we cannot in general say $\Sigma(t_i|\phi) = \phi I_d$.

Clustering

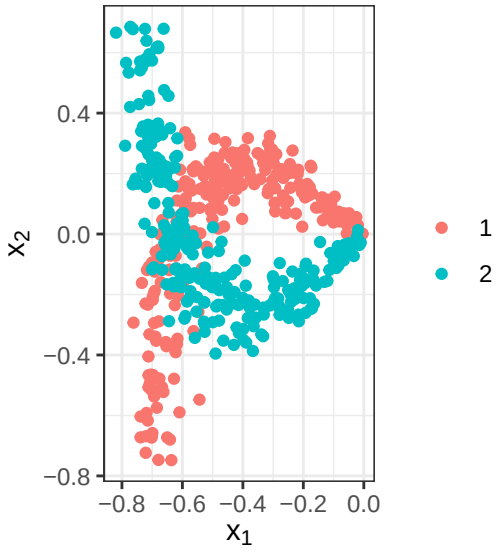
Next, suppose we have K curves parameterized by $g^{(k)}$, with points drawn along these curves. Then one possible clustering technique is as follows:

1. Assign an initial clustering (e.g., via spectral clustering).
2. Estimate the curve for each cluster (using the same curve-fitting procedure as before).
3. Reassign the clusters by proximity to each curve.
4. Repeat 2 and 3 until convergence.

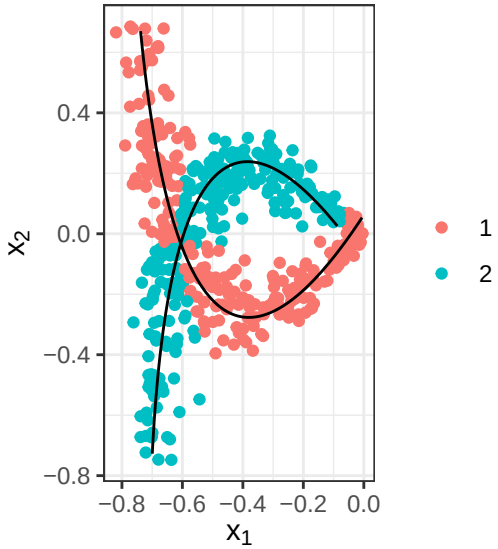
Example 4. *We have two intersecting curves,* $g_1(t) = \begin{bmatrix}t^2 & 2t(1-t)\end{bmatrix}^\top$ *and* $g_2(t) = \begin{bmatrix}2t(1-t) & (1-t)^2\end{bmatrix}^\top$*.* $n_1 = n_2 = 256$ *points are drawn uniformly from each.*



We draw $A \sim \text{RDPG}(X)$ *and obtain the following ASE:*



Fitting two quadratic Bezier curves to these data yields a community detection error rate of 10%. In the following plot, the points are labeled according to their estimated labels.



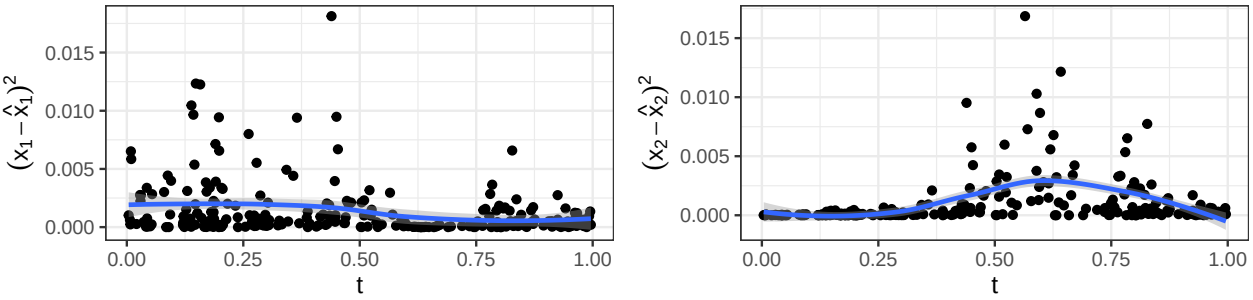
The objective function that this method aims to minimize is:

$$\sum_{k=1}^{K} \sum_{i \in C_k} \|x_i - g(t_i|p_k)\|^2$$

It can be shown that each iteration decreases the objective unless we are at a stationary point.

Model-Based Clustering

The CLT property of the ASE may allow us to approximate $Wx - \hat{x} \sim \mathcal{N}(f_k(t), \Sigma_k)$. One possibly reasonable assumption for Σ_k is $\Sigma_k = \Sigma_k(t) = \text{diag}(\sigma_{k1}^2(t), ..., \sigma_{kd}^2(t))$. A plot of the squared errors of cluster 1 in the previous example reveals the following:



Fitting some curve to each $\sigma_{kr}^2(t)$ allows us to compute estimated probabilities of each point belonging to each cluster/manifold: $\hat{q}_{ik} = \mathcal{N}(x_i \mid g_k(\hat{t}_i), \Sigma_k(\hat{t}_i))$. Then we can use weighted least squares to estimate the parameters of g:

$$\hat{p}_k = (T^\top Q_k T)^{-1} T^\top Q_k X$$

where $Q_k = \text{diag}(q_{1k}, ..., q_{nk})$.