Semi-Parametric Manifold Clustering

Estimating Polynomial Curves

Problem Setup

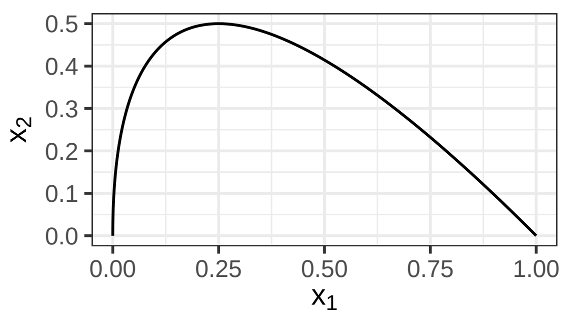
Let:

- $T_1, ..., T_n \stackrel{\text{iid}}{\sim} F$ 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 $g(t) = (t^2, 2t(1-t)) = (t^2, 2t - 2t^2)$. (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., by drawing from a probability distribution).
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.

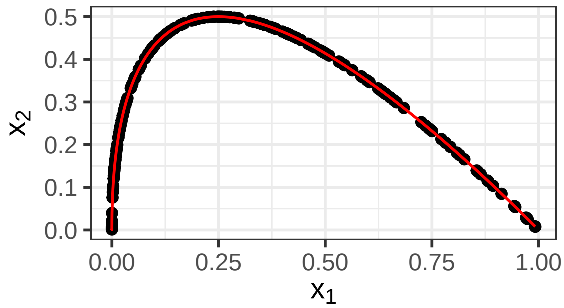
If we restrict g to be polynomials, then steps (2) and (4) have closed-form solutions.

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.

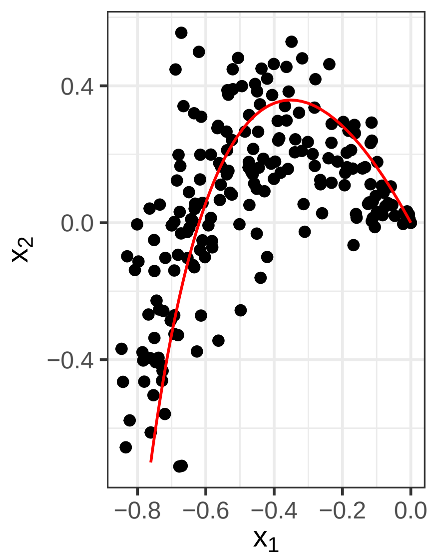
In the following plot, we drew $n = 200$ points from the 2D H-W curve with $T_1, ..., T_n \stackrel{\text{iid}}{\sim} Uniform(0,1)$. The red line is the curve that was fit using the above method.



One problem with this method is the parameterization of the curve is not unique.

Estimation with Noise

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

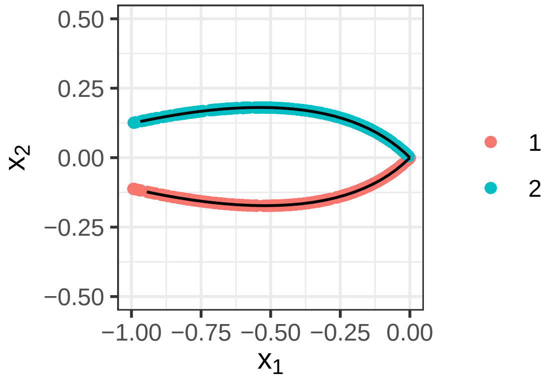


Clustering

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.
3. Reassign the clusters by proximity to each curve.
4. Repeat 2 and 3 until convergence.

Example 4. *We again limit these to be quadratic functions in* $\mathbb{R}^2$*. Here,* $K = 2$ *and* $n_1 = n_2 = 256$*.*



Example 5. *Finally, we draw* $A \sim \mathrm{RDPG}(X)$ *from the above example and apply the clustering and curve fitting to the ASE of* A*.*

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   zhat.manifold
z     1   2
  1 187  69
  2  87 169
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