3.4 The Full Procrustes Mean in a fixed basis

To avoid having to sample the estimated covariance surface $\hat{C}(s,t)$ on a large grid when calculating its leading eigenfunction, it might be preferable to calculate this eigenfunction from the vector of basis coefficients directly.

After choosing a basis representation B with basis functions $b_j(t)$, $j = 1, \dots, k$ we want to estimate coefficients $\theta_j \in \mathbb{C}$ so that the Full Procrustes mean is given by $\hat{\mu}(t) = \sum_{j=1}^{k} \hat{\theta}_j \beta_j(t) = b^T \hat{\theta}$:

$$
\begin{aligned}
\hat{\mu} &= \underset{\theta:||b^T\theta||=1}{\operatorname{argmax}} \sum_{i=1}^{n} \langle b^T\theta, \beta_i \rangle \langle \beta_i, b^T\theta \rangle \\
&= \underset{\theta:||b^T\theta||=1}{\operatorname{argmax}} \sum_{k,l} \sum_{i=1}^{n} \langle b_k\theta_k, \beta_i \rangle \langle \beta_i, b_l\theta_l \rangle \\
&= \underset{\theta:||b^T\theta||=1}{\operatorname{argmax}} \sum_{k,l} \bar{\theta}_k \theta_l \sum_{i=1}^{n} \langle b_k, \beta_i \rangle \langle \beta_i, b_l \rangle \\
&= \underset{\theta:||b^T\theta||=1}{\operatorname{argmax}} \bar{\theta}^T S \theta
\end{aligned}
$$

with $S = \{\sum_{i=1}^{n} \langle b_k, \beta_i \rangle \langle \beta_i, b_l \rangle\}_{k,l}$. As is known from e.g. PCA, the solution to this problem is the leading complex eigenvector $\hat{\theta}$ of the matrix S. We can calculate S in the following way:

$$
\begin{aligned}
S_{kl} &= \sum_{i=1}^{n} \int_0^1 \bar{b}_k(t)\beta_i(t)dt \int_0^1 \bar{\beta}_i(s) b_l(s) ds \\
&= \int_0^1 \int_0^1 \bar{b}_k(t) \underbrace{\left(\sum_{i=1}^{n} \beta_i(t)\bar{\beta}_i(s) \right)}_{=\mathrm{C}(s,t)} b_l(s) ds dt \\
&= \int_0^1 \int_0^1 \bar{b}_k(t) C(s,t) b_l(s) ds dt
\end{aligned}
$$

We may estimate $C(s,t)$ via tensor product splines, so that $\hat{C}(s,t) = \sum_{k,l} \hat{\xi}_{kl} b_k(t) b_l(s)$.

However this does not actually simplify the above expression for S_{kl}:

$$\begin{aligned}
S_{kl} = \cdots = & \int_0^1 \int_0^1 \bar{b}_k(t) \left(\sum_{p,q} \hat{\xi}_{pq} b_q(t) b_p(s) \right) b_l(s) ds dt \\
= & \sum_{p,q} \hat{\xi}_{pq} \int_0^1 \int_0^1 \bar{b}_k(t) b_q(t) b_p(s) b_l(s) ds dt \\
= & \sum_{p,q} \hat{\xi}_{pq} \langle b_k, b_q \rangle \langle \bar{b}_p, b_l \rangle
\end{aligned}$$

At this point we would like to use the properties of an (let's assume orthogonal) basis, so that $\langle b_k, b_q \rangle = \delta_{kq}$, which we can't use here because of the complex conjugate of b_p in the second scalar product. **To solve this nicely wouldn't we need tensor product splines of the form:** $\hat{C}(s,t) = \sum_{k,l} \hat{\xi}_{kl} b_k(t) \bar{b}_l(s)$ **(complex conjugate in the second basis term)?** This would lead us to:

$$\begin{aligned}
S_{kl} = \cdots = & \sum_{p,q} \hat{\xi}_{pq} \langle b_k, b_q \rangle \langle b_p, b_l \rangle \\
= & \sum_{p,q} \hat{\xi}_{pq} \delta_{kq} \delta_{pl} \\
= & \hat{\xi}_{kl}
\end{aligned}$$

Which means the matrix S is just the matrix of coefficients $\hat{\Xi} = \{\hat{\xi}\}_{k,l}$from the covariance smoothing.