Dependently Coupled Principal Component Analysis for Bivariate Inversion Problems

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Contributions

- Propose Dependently Coupled Principal Component Analysis (DC-PCA), to leverage PCA b/w paired datasets in a dependently coupled manner, which is optimal with respect to approximation error during training, applicable to broad class of inversion problems.
    - Often, data contains correlated variables where one is observable to some extent from measurements but other is not observable.
    - Existing methods, CCA/PLSR [1,2], maximize correlation/covariance symmetrically b/w observable & unobservable parts.
    - We generate a dependently coupled paired basis by relaxing orthogonality constraints in decomposing unreliable unobservable measurements.

[1] J. A. Wegelin et al., "A survey of partial least squares (pls) methods, with emphasis on the two-block case," *University of Washington, Tech. Rep,* 2000.
[2] H.Hotelling,"Relations between two sets of variates." *Biometrika*, vol. 28, no. 3/4, pp. 321–377, 1936.

General Inversion Problems

- Critical concept of *raw* data D
  - Entities quantified by various high dimensional measurements (X) and statistics.
  - Dimensions might not be fixed or even finite.
- Computing measurements X directly from D is difficult and expensive.
- Goal of inversion problem is to compute high-dimensional measurement X of raw data D by leveraging low-dimensional representation A (such as PCA expansion coefficients).
- It may be possible to compute A from raw data thus obtaining high-dimensional measurements X via the inverse PCA transform of A.

Independent (Uncoupled PCA)

- Standard PCA applied independently to paired sets (X and Y), yields subspaces which minimize the mean squared error (MSE):

$$\varepsilon(A, U, B, V) = \frac{1}{N}\sum_{n=1}^{N}\left\| \mathrm{x}_n - \underbrace{\sum_{l=1}^{L} \mathrm{u}_l a_{ln}}_{U\mathrm{a}_n} \right\|^2 + \left\| \mathrm{y}_n - \underbrace{\sum_{l=1}^{L} \mathrm{v}_l b_{ln}}_{V\mathrm{b}_n} \right\|^2$$

- The MSE is minimized when we choose U and V as eigenvectors corresponding to largest eigenvalues of XX^T and YY^T respectively.
- The optimal coefficients of expansion are orthogonal projection of data onto respective bases U and V.
- U and V fit data independently without capturing correlations.
- If Y is completely unobservable, then we simply cannot use basis V.

Joint (Symmetrically-Coupled PCA)

- If we allow a single set of expansion coefficients, s.t. the approximations of X and Y must use same set of coefficients then MSE can be written as:

$$\varepsilon(A, U, V) = \frac{1}{N} \sum_{n=1}^{N} \left\| \begin{bmatrix} \mathrm{x}_n \\ \mathrm{y}_n \end{bmatrix} - \sum_{l=1}^{L} \begin{bmatrix} \mathrm{u}_l \\ \mathrm{v}_l \end{bmatrix} a_{ln} \right\|^2$$

- The MSE is minimized when we choose U and V as eigenvectors corresponding to largest eigenvalues of $\begin{bmatrix} X \\ Y \end{bmatrix} \begin{bmatrix} X \\ Y \end{bmatrix}^T$.
- This joint PCA model captures the correlations between the two datasets.
- If Y is completely unobservable during fitting, we get the benefit of correlation, but we don't fit the observable data X optimally.
- Nor does this pairing maximize the correlation b/w the low-dimensional representations of X and Y (as does PLSR)

Dependently Coupled PCA (DC-PCA)

- If again allow a single set of expansion coefficients, A, but impose the standard PCA basis U, together with coefficients A obtained by minimizing MSE for X:

$$\varepsilon_X(A, U) = \frac{1}{N}\sum_{n=1}^{N} \|\mathrm{x}_n - U\mathrm{a}_n\|^2$$

- Now, we may seek a "paired basis" V (not necessarily orthonormal) that minimizes the error term below for this choice of U and A:

$$\varepsilon_Y(A, V) = \frac{1}{N}\sum_{n=1}^{N} \|\mathrm{y}_n - V\mathrm{a}_n^*\|^2$$

- The paired basis V that we seek is given as:

$$V = YX^T U\Lambda_X$$

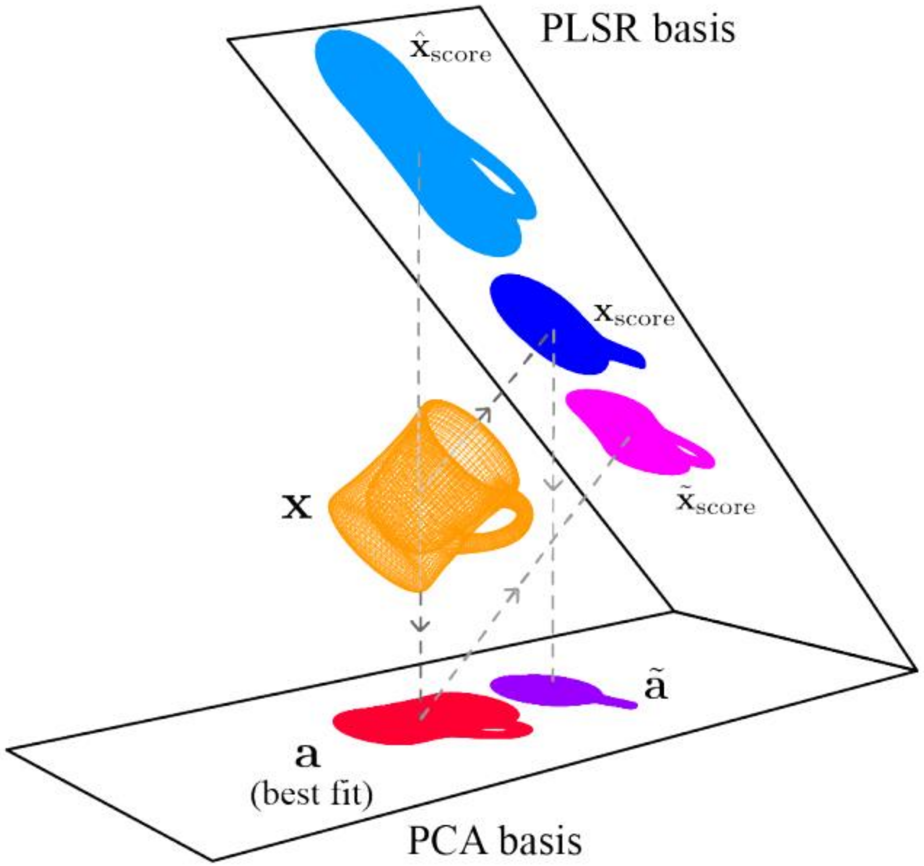
- Λ_X is the diagonal matrix with the largest eigenvalues of XX^T.

Dependently Coupled PCA (DC-PCA)

- Given a set of expansion coefficients which estimate the observable variable X, we may obtain an optimal prediction (according to our training) for an unobservable variable Y by applying the same coefficients to the matching basis elements in V(not necessarily orthonormal).
- This combination of traditional PCA for X, and unidirectional correlation analysis for Y is called Dependently Coupled PCA for the paired data sets.
- The basis V for Y is dependent on the basis U for X, while basis U is completely independent. In this sense the coupling is purely unidirectional.

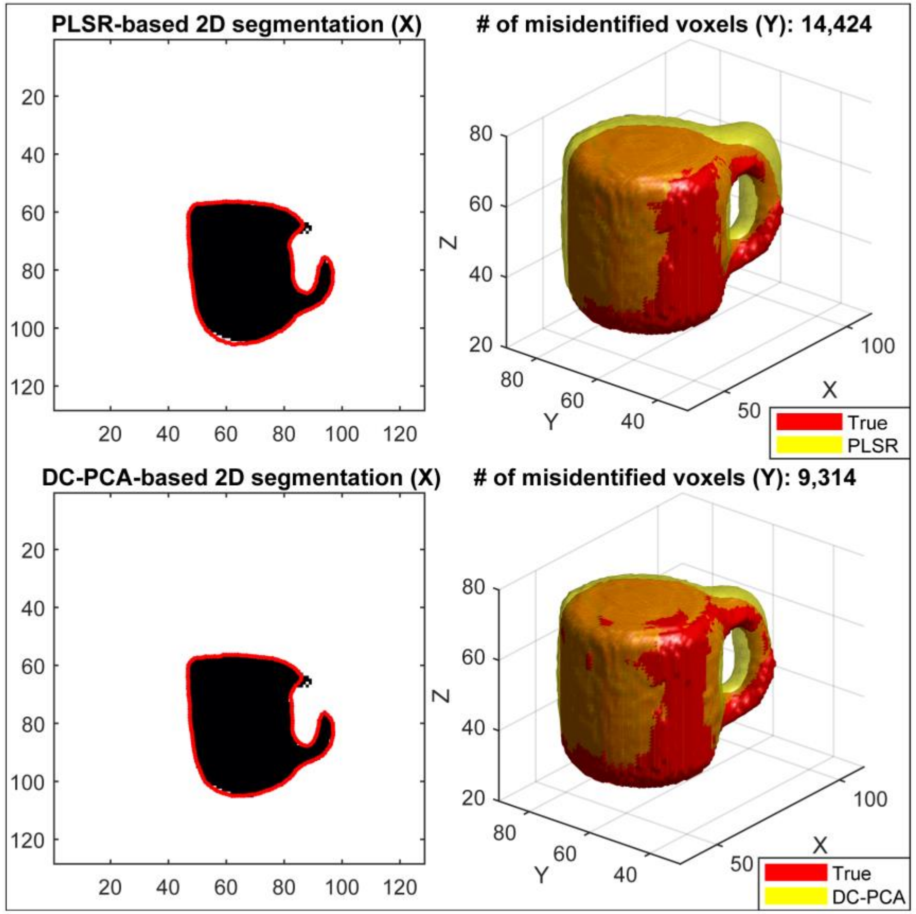
Specialty of DC-PCA for Inversion Problems

- PLS methods (PLSR/CCA) only applicable to prediction problems.
- "Projection of a projection" issue with PLSR in inversion problems: evolution of **a** is driven by the PCA plane.
  - Fit **a** with PCA basis but invert with PLSR basis: only $\tilde{x}_{score}$ (projected from **a**) contributes to the inversion.
  - Fit and invert with PLSR basis: representation $\hat{x}_{score}$(with projection **a** on the PCA plane) does not match the PLSR basis for inversion.



DC-PCA vs PLSR: Synthetic Experiment

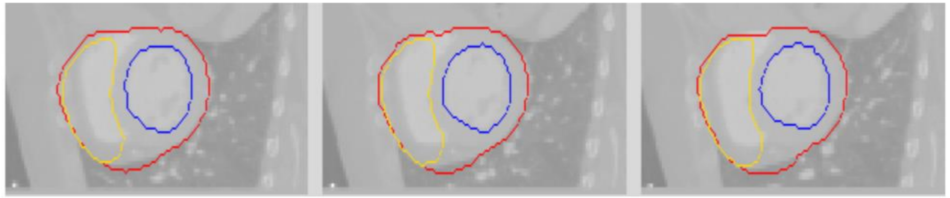
- X represents 2D cross-section shape and Y a paired 3D teacup shape.
- Low dimensional shape inversion is applied to ideal noiseless silhouette using both PCA & PLSR basis for X.
- Both methods extract similar shape from raw image data (left column images).
- However, the estimated 3D surface (Y estimate) from PLSR exhibits higher mismatch against the true shape.

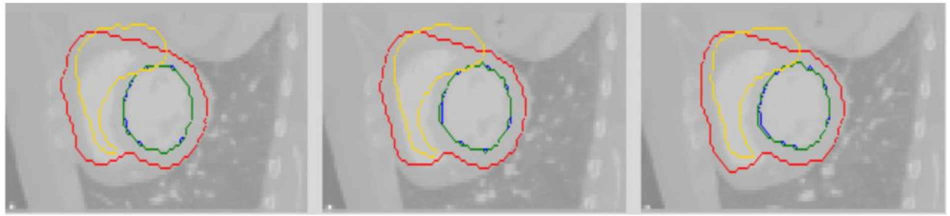


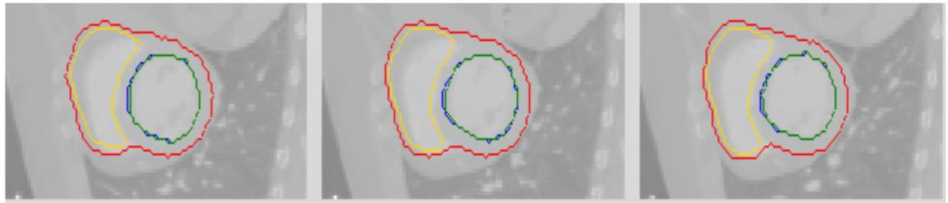
DC-PCA: Practical Application

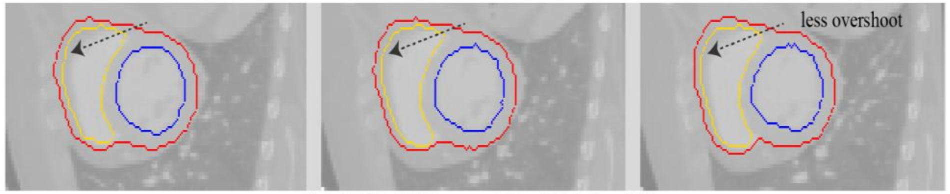
- Objective is to segment the Left Ventricle (LV), Right Ventricle (RV), and Epicardium (EPI) from Cardiac CT imagery using 3D shape models built from manual training segmentations [1].
- LV has good contrast, clear boundaries and hence is easier to segment (observable) compared to RV/EPI (unobservable).
- Estimate RV (yellow) & EPI (red) using DC-PCA based on (fitted) LV (blue) shape coefficients.
- DC-PCA does better in estimating unobservable anatomies (less overshoot in RV compared to PLSR/CCA/Joint PCA).

[1] N. Dahiya, A. Yezzi, M. Piccinelli, E. Garcia, "Integrated 3D Anatomical Model for Automatic Segmentation in Cardiac CT Imagery", *Computer Methods in Biomechanics & Biomedical Imagery*, 2019


(a) Joint PCA (symmetrically paired) DICE scores: RV = 0.61, EPI = 0.87


(b) CCA DICE scores: RV = 0.40 EPI = 0.89


(c) PLSR DICE scores: RV = 0.65 EPI = 0.91



(d) DC-PCA DICE scores: RV = 0.75 EPI = 0.93

Conclusions

- Presented a novel method of leveraging PCA between paired datasets, in a unidirectional, dependently-coupled manner.
- Optimal with respect to approximation error during training.
- Specially customized for broad class of inversion problems with better suitability than existing methods.