Semi-supervised Kernel Canonical Correlation Analysis of Human Functional Magnetic Resonance Imaging Data

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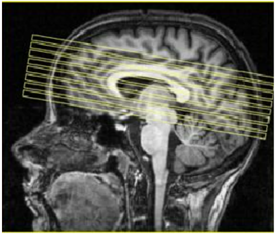
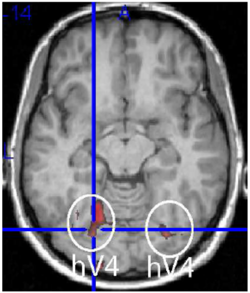
Introduction

Motivation

- **Neuroscience: assess natural processing**, i.e. fMRI – reduce dimensions to main activity during shown stimulus



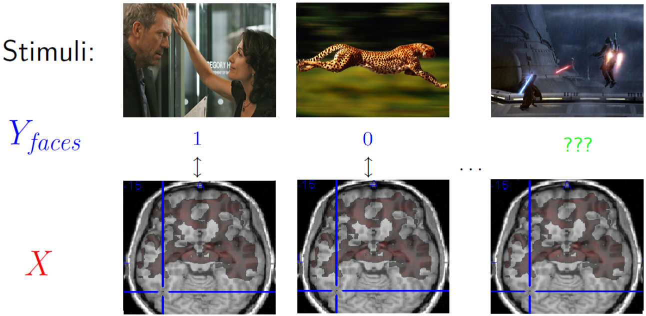


- **Problems:** high-dimensional data, expensive labels
- **Goal:** Canonical Correlation Analysis in semi-supervised learning framework

Paired Data

- Samples in **2 modalities**: representations of 1 process,
  $\longrightarrow$ labeled video shown during fMRI acquisition

Illustration:

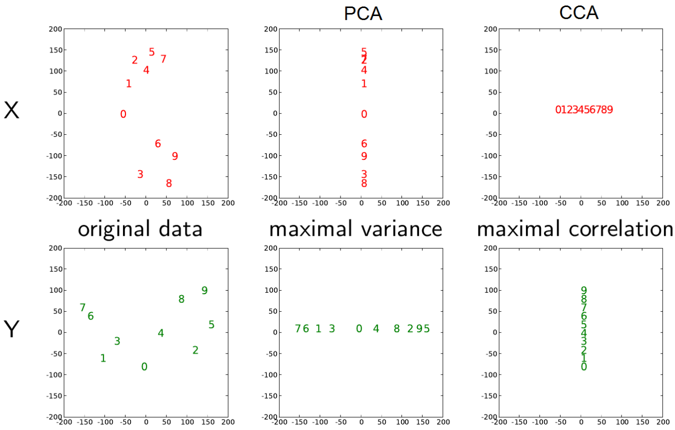


fMRI data: (labeled) $X = \{x_1, x_2, \ldots, x_n\}$, (unlabeled) $\{x_{n+1}, \ldots, x_p\}$
Corresponding labels: $Y = \{y_1 = 1, y_2 = 0, \ldots, y_n\}$

$\longrightarrow$ Paired data (fMRI with labels): $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$

Canonical Correlation Analysis (CCA)

- Finds projection directions in each modality's subspace that **maximize correlation** between the projected data
  $\longrightarrow$ Not directions of (potentially noisy) maximal variance



Kernel Canonical Correlation Analysis

- **CCA:** maximize correlation between X and Y projections

Optimize CCA e.g. as a generalized eigenvalue problem:

$$\max_{w_x, w_y} \quad \frac{w_x^T C_{xy} w_y}{\sqrt{(w_x^T C_{xx} w_x)(w_y^T C_{yy} w_y)}} \tag{1}$$

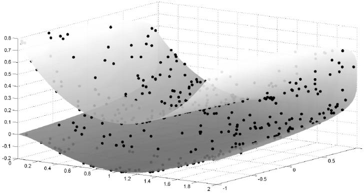
- **Kernelized CCA (KCCA)**: general, optimization easier
- **Regularized KCCA**: avoid degenerate solutions

Optimize Tikhonov regularized KCCA:

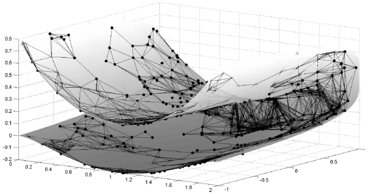
$$\max_{\alpha, \beta} \frac{\alpha^T K_x K_y \beta}{\sqrt{\alpha^T \left(K_x^2 + \varepsilon_x K_x\right) \alpha \beta^T \left(K_y^2 + \varepsilon_y K_y\right) \beta}} \tag{2}$$

Manifold assumption

- **Manifold assumption**: high-dimensional data lie on a low-dimensional manifold $\mathcal{M}$ (Belkin et al., 2006)
- Functions should vary smoothly along $\mathcal{M}$ – small gradient
- Estimate the gradient $\nabla_{\mathcal{M}}$ by constructing a graph along the manifold $\mathcal{M}$:



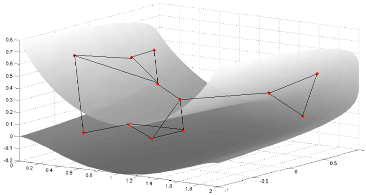
Samples of manifold



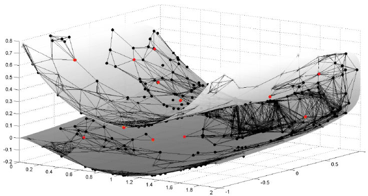
Graph estimate of manifold

Laplacian Regularization

- Gradient estimate $\nabla_{\mathcal{M}}$ of functions along $\mathcal{M}$ leads to **Laplacian regularization** – adding term $\mathcal{L}$ to optimization enforces smoothness along the manifold
- Optionally unlabeled data can be included to improve estimate of manifold $\rightarrow$ **semi-supervised**



Poor estimate: Graph with few data points



Better estimate: Graph with more data points

Laplacian regularized SSKCCA:

$$\max_{\alpha,\beta} \frac{\alpha^T K_{\hat{x}x} K_{yy} \beta}{\sqrt{\alpha^T \left(K_{\hat{x}x} K_{x\hat{x}} + R_{\hat{x}}\right) \alpha \beta^T \left(K_y^2\right) \beta}}, \tag{3}$$

with regularizers

$$R_{\hat{x}} = \underbrace{\varepsilon_x K_{\hat{x}\hat{x}}}_{\text{Tikhonov}} + \underbrace{\frac{\gamma_x}{m_x^2} K_{\hat{x}\hat{x}} \mathcal{L}_{\hat{x}} K_{\hat{x}\hat{x}}}_{\text{Laplacian}}$$

- SSKCCA will favor directions α and β whose projections are **smooth along the manifold** (Blaschko et al., 2008)

- **fMRI data (X):** human volunteer during viewing of 2 movies
  - 350 time slices of 3D fMRI brain volumes per movie
- **Labels (Y):** Continuous labels, 1 movie – 5 observers' scores:
  Faces - Color - Bodies - Language - Motion (Bartels and Zeki 2004)
- **Linear kernel** in all experiments

Experiments

(a) KCCA with Tikhonov regularization
$\longrightarrow$ labeled data only

(b) KCCA with Tikhonov and Laplacian regularization
$\longrightarrow$ labeled data only

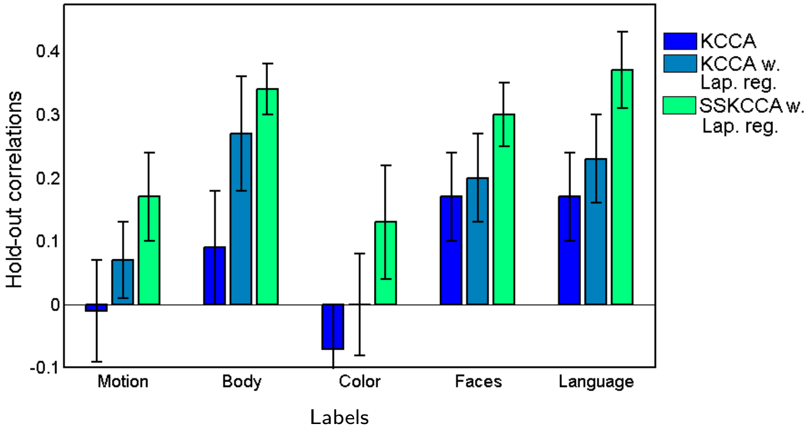
(c) SSKCCA with Tikhonov and Laplacian regularization
$\longrightarrow$ labeled and unlabeled data

- **Model Selection**: criterion from (Hardoon et al., 2004) to optimize over the regularization parameters (ε_x and γ_x)

Experiments

Results – Quantitative

Mean holdout correlations from five-fold cross validation across [each of the five] variables in all experiments.

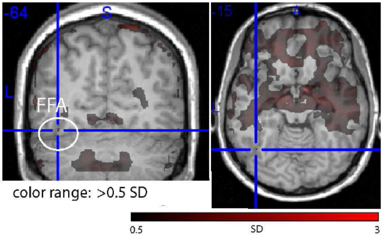


→ SSKCCA generalizes better than KCCA

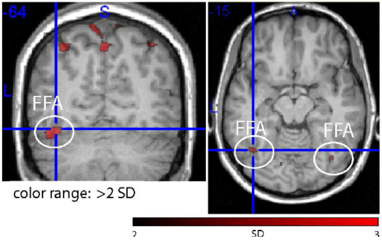
Experiments

Results – Qualitative

Visualization of learned weight vectors for faces



KCCA, Tikhonov regularization



SSKCCA, Tikhonov and Laplacian regularization

$\longrightarrow$ SSKCCA localizes regions of brain activity, following (Bartels and Zeki, 2004)

Summary

- SSKCCA learned expected regions of brain activity corresponding to input stimuli (Bartels and Zeki, 2004)
- KCCA with Laplacian regularization improves correlation by enforcing smoothness of projections along the manifold
- SSKCCA with use of unlabeled data further improves performance
- Check out **poster M26** for our extension of this work using resting state fMRI data as an unlabeled data source

Summary

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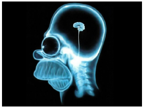
Thanks.



Appendix – References

1. Bartels, A., Zeki, S., and Logothetis, N. K. (2008). Natural vision reveals regional specialization to local motion and to contrast-invariant, global flow in the human brain. Cereb Cortex 18:705-717.
2. Bartels, A., Zeki, S. (2004). The chronoarchitecture of the human brain - natural viewing conditions reveal a time-based anatomy of the brain. NeuroImage 22:419-433.
3. Belkin, M., Niyogi, P., Sindhwani, V.: Manifold Regularization: A Geometric Framework for Learning from Labeled and Unlabeled Examples. JMLR (2006)
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Appendix

Kernelization

$$\max_{w_x, w_y} \frac{w_x^T C_{xy} w_y}{\sqrt{w_x^T C_{xx} w_x \; w_y^T C_{yy} w_y}}. \tag{4}$$

We denote $\mathcal{H}_x$ the reproducing kernel Hilbert space (RKHS) associated with k_x, and denote the associated feature map $\phi_x : \mathcal{X} \to \mathcal{H}$, i.e. $k_x(x_i, x_j) = \langle \phi_x(x_i), \phi_x(x_j) \rangle$.

$$\max_{f_x, f_y} \frac{f_x^T \hat{C}_{xy} f_y}{\sqrt{f_x^T \hat{C}_{xx} f_x \; f_y^T \hat{C}_{yy} f_y}} = \max_{\alpha, \beta} \frac{\alpha^T K_x K_y \beta}{\sqrt{\alpha^T K_x^2 \alpha \; \beta^T K_y^2 \beta}}, \tag{5}$$

$$\max_{\alpha, \beta} \frac{\alpha^T K_x K_y \beta}{\sqrt{\alpha^T \left(K_x^2 + \varepsilon_x K_x\right) \alpha \beta^T \left(K_y^2 + \varepsilon_y K_y\right) \beta}}, \tag{6}$$

Denoting the kernel matrix computed using the data in X as $K_{xx} \in \mathbb{R}^{n \times n}$, the matrix computed using $\hat{X}$ and X as $K_{\hat{x}x} \in \mathbb{R}^{m_x \times n}$, the matrix computed using $\hat{X}$ with itself as $K_{\hat{x}\hat{x}} \in \mathbb{R}^{m_x \times m_x}$, etc. Kernel matrices for $\mathcal{Y}$ can be defined analogously.
Semi-supervised Laplacian regularized generalization of above equation:

$$\max_{\alpha, \beta} \frac{\alpha^T K_{\hat{x}x} K_{y\hat{y}} \beta}{\sqrt{\alpha^T \left(K_{\hat{x}x} K_{x\hat{x}} + R_{\hat{x}}\right) \alpha \beta^T \left(K_{\hat{y}y} K_{y\hat{y}} + R_{\hat{y}}\right) \beta}}, \tag{7}$$

Graph Laplacian term $\mathcal{L}$:

$$\mathcal{L} = D^{-1/2}(D - W)D^{-1/2}$$

where W is the matrix of similarities between data points
and D is the diagonal matrix with entries of W's row sums

for similarity kernel $(K)_{ij} = \exp\left(\frac{-\|x_i - x_j\|^2}{\sigma^2}\right)$
and diagonal of row sums $(D_{\hat{x}\hat{x}})_{ii} = \sum_{j=1}^{n+p_x}(K_{\hat{x}\hat{x}})_{ij}$.

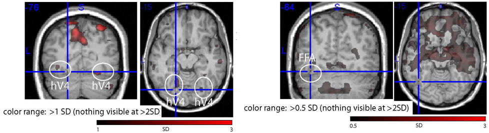
Appendix

Data and Acquisition

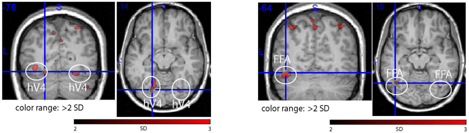
- fMRI data of one human volunteer during viewing of 2 movies.
- 350 time slices of 3-dimensional fMRI brain volumes acquired with Siemens 3T TIM scanner, separated by 3.2 s (TR), with a spatial resolution of 3x3x3 mm.
- Pre-processed according to standard procedures using the Statistical Parametric Mapping (SPM) toolbox [6].

Visualization of learned weight vectors (w_x) for color and face stimuli, following [2].

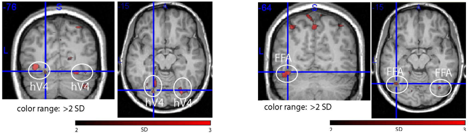
Color Faces



(a) CCA, Tikhonov regularization

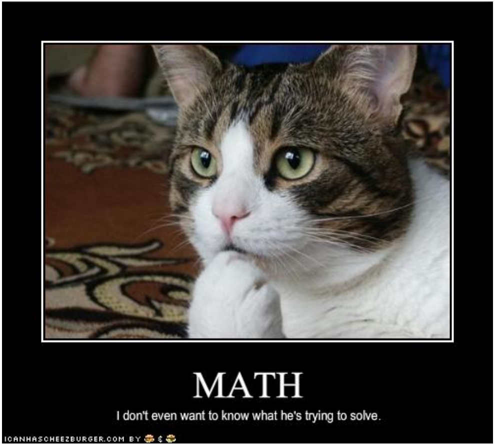


(b) CCA, Tikhonov and Laplacian regularization



(c) Semi-supervised CCA, Tikhonov and Laplacian regularization

Just a kitty


MATH
I don't even want to know what he's trying to solve.
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