Deflation Methods for Sparse PCA

Lester Mackey

Background

Principal Components Analysis (PCA)

- **Goal:** Extract r leading eigenvectors of sample covariance matrix, A_0
- **Typical solution:** Alternate between two tasks
  1. Rank-one variance maximization
     $x_t = \arg\max x^T A_{t-1} x \text{ s.t. } x^T x = 1$
  2. Hotelling's matrix deflation
     $A_t = A_{t-1} - x_t x_t^T A_{t-1} x_t x_t^T$
     - Removes contribution of x_t from A_{t-1}
- **Primary drawback:** Non-sparse solutions

Sparse PCA

- **Goal:** Extract r sparse "pseudo-eigenvectors"
  - High variance directions, few non-zero components
- **Typical solution:** Alternate between two tasks
  1. Constrained rank-one variance maximization
     $x_t = \arg\max x^T A_{t-1} x \text{ s.t. } x^T x = 1, \text{Card}(x) \le k_t$
  2. Hotelling's matrix deflation (borrowed from PCA)

The Problem

Hotelling's deflation was designed for eigenvectors, not pseudo-eigenvectors

Compare

- **Hotelling's deflation for PCA**
  - Annihilates variance of x_t: $x_t^T A_t x_t = 0$
  - Renders A_t orthogonal to x_t: $A_t x_t = 0$
  - Preserves positive semidefiniteness: $A_t \succeq 0$
- **Hotelling's deflation for Sparse PCA**
  - Annihilates variance of x_t
  - **Does not render A_t orthogonal to x_t**
  - **Does not preserve positive semidefiniteness**

Key properties lost in the Sparse PCA setting

Goal: Recover lost properties with new deflation methods

Alternative Deflation Methods

Projection Deflation

$$A_t = (I - x_t x_t^T) A_{t-1} (I - x_t x_t^T)$$

Intuition: Projects data onto orthocomplement of space spanned by x_t

Schur Complement Deflation

$$A_t = A_{t-1} - \frac{A_{t-1} x_t x_t^T A_{t-1}}{x_t^T A_{t-1} x_t}$$

Intuition: Conditional variance of data variables given the new sparse principal component

Orthogonalized Projection Deflation

$$q_t = \frac{(I - Q_{t-1} Q_{t-1}^T) x_t}{\| (I - Q_{t-1} Q_{t-1}^T) x_t \|}, A_t = (I - q_t q_t^T) A_{t-1} (I - q_t q_t^T)$$

Intuition: Eliminates *additional* variance contributed by x_t

- Q_t = orthonormal basis for extracted pseudo-eigenvectors
- Successive pseudo-eigenvectors are not orthogonal
- Annihilating full vector can reintroduce old components
- Orthogonalized Hotelling's Deflation defined similarly

Reformulating Sparse PCA

New goal: Explicitly maximize additional variance criterion

- Solve sparse generalized eigenvector problem
  $$\max_x x^T (I - Q_{t-1} Q_{t-1}^T) A_0 (I - Q_{t-1} Q_{t-1}^T) x$$
  $$\text{s.t. } x^T (I - Q_{t-1} Q_{t-1}^T) x = 1, \text{Card}(x) \le k_t$$
- Yields generalized deflation procedure

Generalized Deflation

$$q_t = B_{t-1} x_t, \ B_t = B_{t-1}(I - q_t q_t^T)$$

$$A_t = (I - q_t q_t^T) A_{t-1} (I - q_t q_t^T)$$

Deflation Properties

Method	$x_t^T A_t x_t = 0$	$A_t x_t = 0$	$A_t \succeq 0$	$A_s x_t = 0, \forall s > t$
Hotelling's (HD)	√	X	X	X
Projection (PD)	√	√	√	X
Schur Complement (SCD)	√	√	√	√
Orthog. Hotelling's (OHD)	√	X	X	X
Orthog. Projection (OPD)	√	√	√	√
Generalized (GD)	√	√	√	√

Experiments

Set up: Leading deflation-based Sparse PCA algorithms

- GSLDA (Moghaddam et al., ICML '06)
- DC-PCA (Sriperumbudur et al., ICML '07)
- Outfitted with each deflation technique

Pit props dataset: 13 variables, 180 observations

DC-PCA Cumulative % variance, Cardinality 4,4,4,4,4,4

	HD	PD	SCD	OHD	OPD	GD
PC 1	22.60%	22.60%	22.60%	22.60%	22.60%	22.60%
PC 2	39.60%	39.60%	38.60%	39.60%	39.60%	39.60%
PC 3	46.80%	50.90%	53.40%	46.80%	50.90%	51.00%
PC 4	56.80%	62.10%	62.30%	52.90%	62.10%	62.20%
PC 5	66.10%	70.20%	73.70%	59.90%	70.20%	71.30%
PC 6	73.40%	77.80%	79.30%	63.20%	77.20%	78.90%

Gene expression dataset: 21 genes, 5759 fly nuclei

GSLDA Cumulative % variance, Cardinality 9,7,6,5,3,2,2,2

	HD	PD	SCD	OHD	OPD	GD
PC 1	21.00%	21.00%	21.00%	21.00%	21.00%	21.00%
PC 2	38.20%	38.10%	38.10%	38.20%	38.10%	38.20%
PC 3	52.10%	51.90%	52.00%	52.00%	51.90%	52.20%
PC 4	60.50%	60.60%	60.40%	60.40%	60.40%	61.00%
PC 5	65.70%	67.40%	67.10%	65.90%	67.10%	68.20%
PC 6	69.30%	71.00%	70.40%	70.00%	70.00%	72.10%
PC 7	72.50%	74.00%	73.40%	72.80%	73.70%	75.70%
PC 8	75.10%	76.80%	77.00%	75.90%	76.60%	79.60%