Fast algorithms for sparse principal component analysis based on Rayleigh quotient iteration

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Sparse principal component analysis

Seeks principal components that maximize variance subject to a sparsity constraint:

Sparse PCA	PCA
$$\begin{aligned} \max \quad & \frac{1}{2} x^T \Sigma x \\ \text{s.t.} \quad & \|x\|_2 \leq 1 \\ & \|x\|_0 \leq k \end{aligned}$$	$$\begin{aligned} \max \quad & \frac{1}{2} x^T \Sigma x \\ \text{s.t.} \quad & \|x\|_2 \leq 1 \end{aligned}$$

where $\Sigma \in \mathbb{R}^{n \times n}$, $\Sigma = \Sigma^T$ and $k > 0$.

Current state-of-the-art

The most successful methods are variations of the *generalized power method*.

Algorithm 1 GPM(Σ, x_0, γ, ϵ)

$j \leftarrow 0$
repeat
  $y \leftarrow \Sigma x^{(j)}$
  $x^{(j+1)} \leftarrow \mathrm{SparsifyAndScale}_\gamma(y)$ // New relative to pow. met.
  $j \leftarrow j + 1$
until $||x^{(j)} - x^{(j-1)}|| < \epsilon$

return $x^{(j)}$

The sparsification step typically consists of soft thresholding and scaling to a norm of one.

Rayleigh quotient iteration

A more sophisticated algorithm for computing eigenvalues than the power method.

Algorithm 2 RayleighQuotientIteration(Σ, x_0, ϵ)

$j \leftarrow 0$
repeat
  $\mu \leftarrow \dfrac{(x^{(j)})^T \Sigma x^{(j)}}{(x^{(j)})^T x^{(j)}}$ // Rayleigh quotient

  $x^{(j+1)} \leftarrow \dfrac{(\Sigma - \mu I)^{-1} x^{(j)}}{||(\Sigma - \mu I)^{-1} x^{(j)}||}$

  $j \leftarrow j + 1$
until $||x^{(j)} - x^{(j-1)}|| < \epsilon$
return $x^{(j)}$

Generalized Rayleigh quotient iteration

Algorithm 3 GRQI(Σ, x_0, k, J, ϵ)

$j \leftarrow 0$
repeat
  $\mathcal{W} \leftarrow \{i | x_i^{(j)} \neq 0\}$
  $x_{\mathcal{W}}^{(j)} \leftarrow \mathrm{RQIStep}(x_{\mathcal{W}}^{(j)}, \Sigma_{\mathcal{W}})$ // Rayleigh quotient update

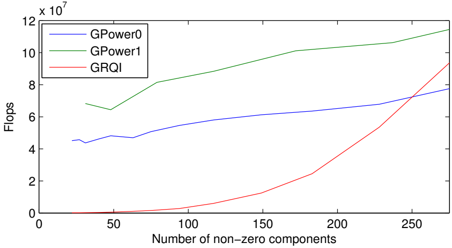
  if $j < J$ **then**
    $x^{(j)} \leftarrow \Sigma x^{(j)} / ||\Sigma x^{(j)}||_2$ // Power met. update
  end if

  $x^{(j+1)} \leftarrow \mathrm{Project}_k\,(x_{\mathrm{new}})$ // Project on $l_0 \cap l_2$ ball.
  $j \leftarrow j + 1$
until $||x^{(j)} - x^{(j-1)}|| < \epsilon$
return $x^{(j)}$

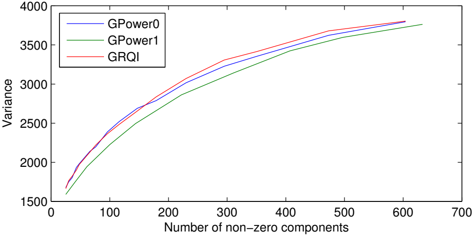
Comparison

Gen. power method	**Gen. Rayleigh quotient iter.**
Extends power method	Extends Rayleigh quotient iter.
Form of gradient descent	A second-order method
Linear convergence	Cubic convergence
$O(nk + n^2)$ flops per iter.	$O(nk + k^3)$ flops per iter.
Converges in about 100 iter.	Converges in about 10 iter.

Comparison



(a) Flops to compute eigenvector as a function of sparsity ($\mathbb{R}^{1000\times1000}$)



(b) Variance/sparsity tradeoff (random matrices in $\mathbb{R}^{1000\times1000}$)

Summary

New algorithms for sparse PCA that

- Use 10-100x fewer flops than the best current methods;
- Find sparse components which are as good or better than ones from existing algorithms;
- Generalize Rayleigh quotient iteration.

This motivates further research into second-order methods for doing matrix factorizations.