COMPSCI 514: Algorithms for Data Science

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University of Massachusetts Amherst. Fall 2022.

Lecture 21

Logistics

- Quiz due Monday at 8pm.
- No class next week – Friday schedule is followed on Tuesday.
- Regular office hours on Tuesday.
- Pset 4 released by end of week.
- Pset 5 short, EC

Summary

Last Few Classes: Spectral Graph Partitioning

- Focus on separating graphs with small but relatively balanced cuts.
- Connection to second smallest eigenvector of graph Laplacian.
- Provable guarantees for stochastic block model.
- Expectation analysis in class. See slides for full analysis.

This Class: Computing the SVD/eigendecomposition.

- Efficient algorithms for SVD/eigendecomposition.
- Iterative methods: power method, Krylov subspace methods.
- High level: a glimpse into fast methods for linear algebraic computation, which are workhorses behind data science.

Efficient Eigendecomposition and SVD

We have talked about the eigendecomposition and SVD as ways to compress data, to embed entities like words and documents, to compress/cluster non-linearly separable data.

How efficient are these techniques? Can they be run on large datasets?

Computing the SVD

Basic Algorithm: To compute the SVD of full-rank $\mathbf{X} \in \mathbb{R}^{n \times d}$, $\mathbf{X} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$:

- Compute $\mathbf{X}^T\mathbf{X}$ – $O(nd^2)$ runtime.
- Find eigendecomposition $\mathbf{X}^T\mathbf{X} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^T$ – $O(d^3)$ runtime.
- Compute $\mathbf{L} = \mathbf{X}\mathbf{V}$ – $O(nd^2)$ runtime. Note that $\mathbf{L} = \mathbf{U}\mathbf{\Sigma}$.
- Set $\sigma_i = \|\mathbf{L}_i\|_2$ and $\mathbf{U}_i = \mathbf{L}_i / \|\mathbf{L}_i\|_2$. – $O(nd)$ runtime.

Total runtime: $O(nd^2 + d^3) = O(nd^2)$ (assume w.l.o.g. $n \geq d$)

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- The worlds fastest super computers compute at ≈ 100 petaFLOPS = 10^{17} FLOPS (floating point operations per second).
- This is a relatively easy task for them – but no one else.

Faster Algorithms

To speed up SVD computation we will take advantage of the fact that we typically only care about computing the top (or bottom) k singular vectors of a matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$ for $k \ll d$.

- Suffices to compute $\mathbf{V}_k \in \mathbb{R}^{d \times k}$ and then compute $\mathbf{U}_k \mathbf{\Sigma}_k = \mathbf{X}\mathbf{V}_k$.
- Use an *iterative algorithm* to compute an *approximation* to the top k singular vectors $\mathbf{V}_k$ (the top k eigenvectors of $\mathbf{X}^T\mathbf{X}$.)
- Runtime will be roughly $O(ndk)$ instead of $O(nd^2)$.

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Sparse (iterative) vs. Direct Method. `svd` vs. `svds`.

eig eigs

Power Method

Power Method: The most fundamental iterative method for approximate SVD/eigendecomposition. Applies to computing $k = 1$ eigenvectors, but can be generalized to larger k.

Goal: Given symmetric $\mathbf{A} \in \mathbb{R}^{d \times d}$, with eigendecomposition $\mathbf{A} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^T$, find $\vec{z} \approx \vec{v}_1$. I.e., the top eigenvector of $\mathbf{A}$.

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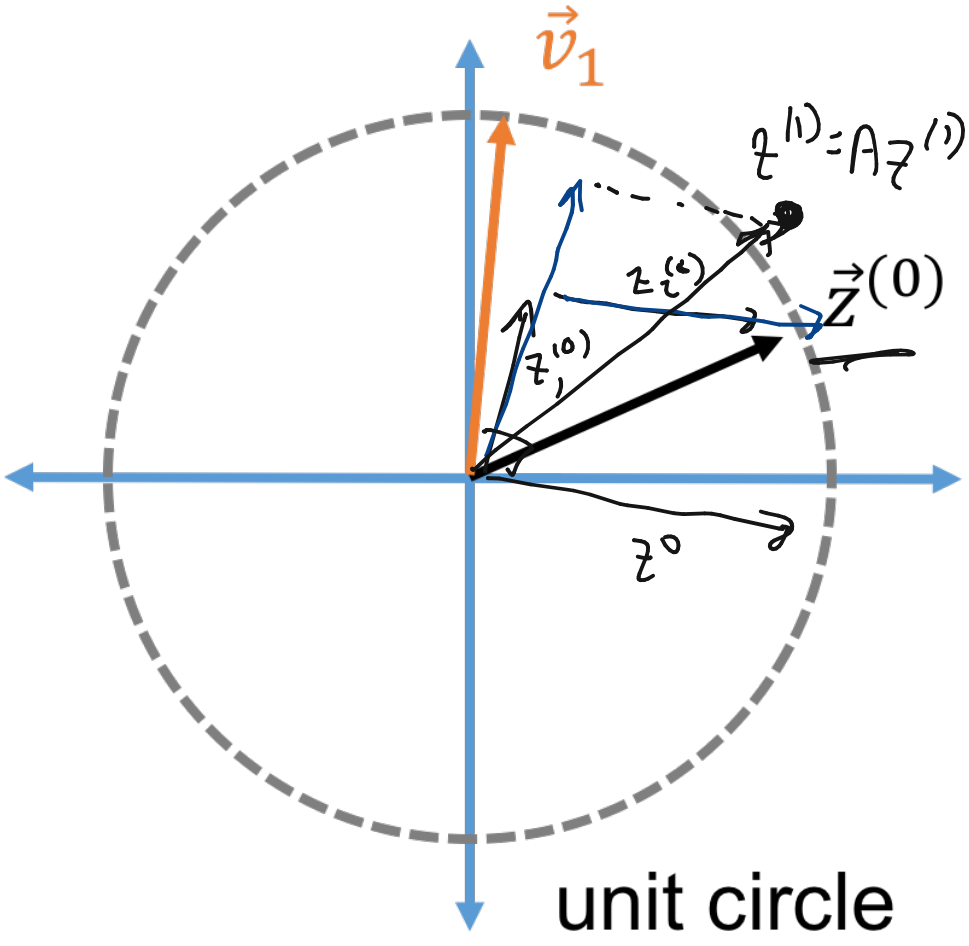
- **Initialize:** Choose $\vec{z}^{(0)}$ randomly. E.g. $\vec{z}^{(0)}(i) \sim \mathcal{N}(0, 1)$.
- For $i = 1, \ldots, t$
  - $\vec{z}^{(i)} := \mathbf{A} \cdot \vec{z}^{(i-1)}$
  - $\vec{z}_i := \frac{\vec{z}^{(i)}}{\|\vec{z}^{(i)}\|_2}$

  Return $\vec{z}_t$

Power Method

$\left[A \right]^2$

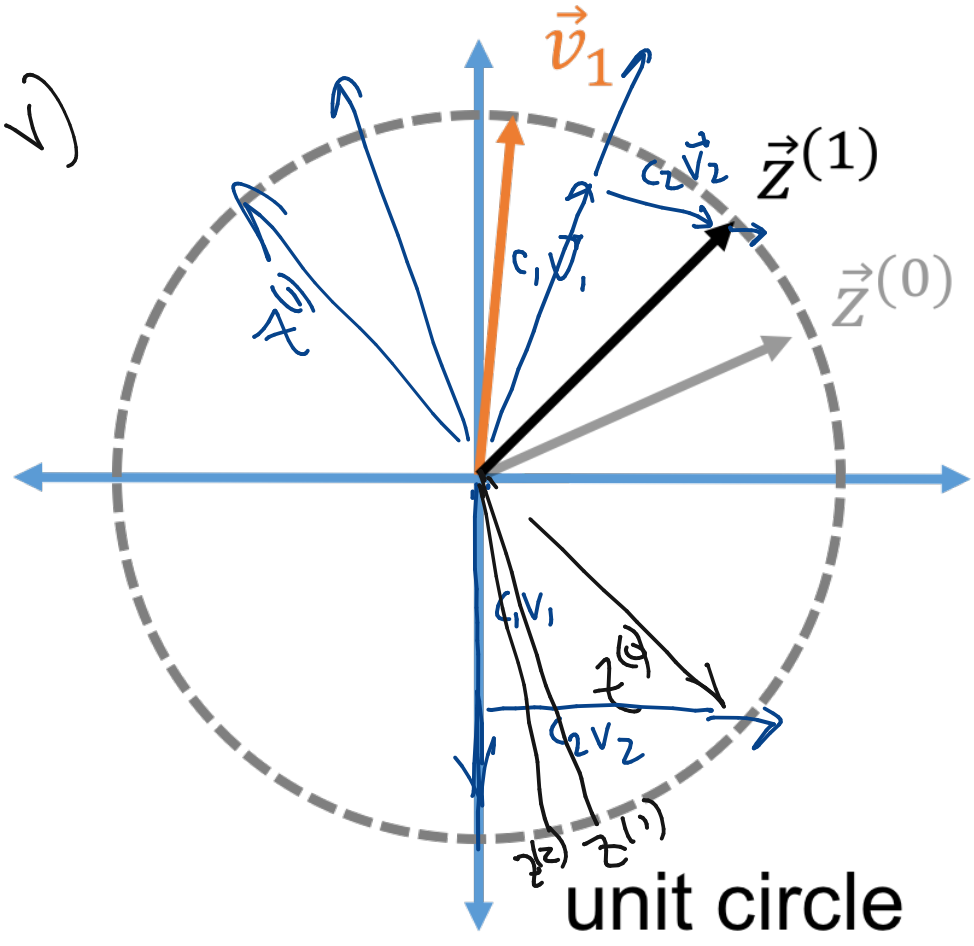
$z^{(1)} = Az^{(0)}$



Power Method

$Av = \lambda v$

$A(-v) = \lambda(-v)$



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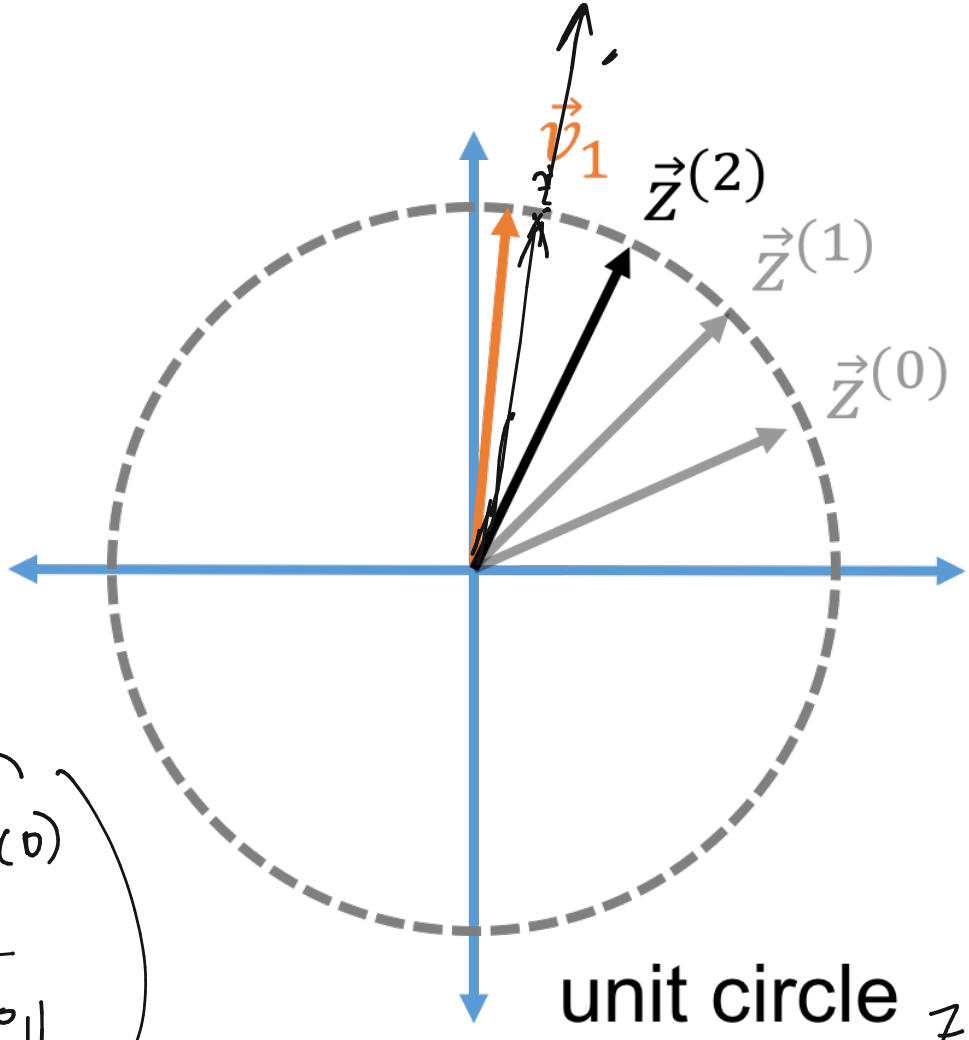

$$A\left(\|Az^{(0)}\|\,\frac{Az^{(0)}}{\|Az^{(0)}\|}\right) = \underbrace{z^{(1)}}$$

$$\|Az^{(0)}\| \cdot A \cdot z^{(1)} = \underbrace{\|Az^{(0)}\| \cdot \|Az^{(1)}\|}_{} \cdot \underbrace{\frac{Az^{(1)}}{\|Az^{(1)}\|}}_{z^{(2)}}$$

Power Method Analysis

Write $\vec{z}^{(0)}$ in $\mathbf{A}$'s eigenvector basis:

$$\vec{z}^{(0)} = c_1\vec{v}_1 + c_2\vec{v}_2 + \ldots + c_d\vec{v}_d.$$

$\mathbf{A} \in \mathbb{R}^{d\times d}$: input matrix with eigendecomposition $\mathbf{A} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^T$. $\vec{v}_1$: top eigenvector, being computed, $\vec{z}^{(i)}$: iterate at step i, converging to $\vec{v}_1$.

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Update step: $\vec{z}^{(i)} = \mathbf{A} \cdot \vec{z}^{(i-1)} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^T \cdot \vec{z}^{(i-1)}$ (then normalize)

$$\mathbf{V}^T\vec{z}^{(0)} = \begin{bmatrix} \vec{v}_1^T \\ \vec{v}_2^T \\ \vdots \\ \vec{v}_d^T \end{bmatrix} \begin{bmatrix} \\ z^0 \\ \\ \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_d \end{bmatrix}$$

$$\vec{v}_i^T z^0$$

$$\vec{v}_i^T(c_1\vec{v}_1 + c_2\vec{v}_2 \ldots + c_d\vec{v}_d)$$

$$= c_i\vec{v}_i^T\vec{v}_i = c_i$$

$$\mathbf{\Lambda}\mathbf{V}^T\vec{z}^{(0)} = \begin{bmatrix} \lambda_1 c_1 \\ \lambda_2 c_2 \\ \vdots \\ \lambda_d c_d \end{bmatrix}$$

$$\vec{z}^{(1)} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^T \cdot \vec{z}^{(0)} = \begin{bmatrix} | & & | \\ \vec{v}_1 & \cdots & \vec{v}_d \\ | & & | \end{bmatrix} \begin{bmatrix} \lambda_1 c_1 \\ \vdots \\ \lambda_d c_d \end{bmatrix} = \lambda_1 c_1 \vec{v}_1 + \lambda_2 c_2 \vec{v}_2 + \ldots \lambda_d c_d \vec{v}_d$$

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Claim 2:

$$\vec{z}^{(t)} = c_1 \cdot \lambda_1^t\vec{v}_1 + c_2 \cdot \lambda_2^t\vec{v}_2 + \ldots + c_d \cdot \lambda_d^t\vec{v}_d.$$

1.1^{50}

$z^{(t)} \approx v_1$

$\lambda_1^t \gg \lambda_2^t \gg \lambda_3^t \ldots$

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Power Method Convergence

After t iterations, we have 'powered' up the eigenvalues, making the component in the direction of v_1 much larger, relative to the other components.

$$\vec{z}^{(0)} = c_1\vec{v}_1 + c_2\vec{v}_2 + \ldots + c_d\vec{v}_d \implies \vec{z}^{(t)} = c_1\lambda_1^t\vec{v}_1 + c_2\lambda_2^t\vec{v}_2 + \ldots + c_d\lambda_d^t\vec{v}_d$$

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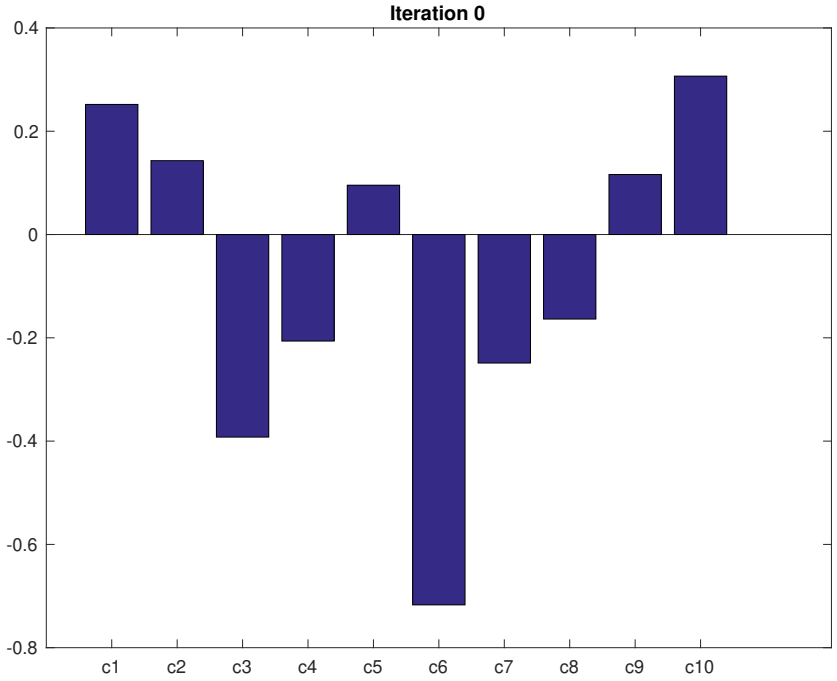
$z^{(0)}$



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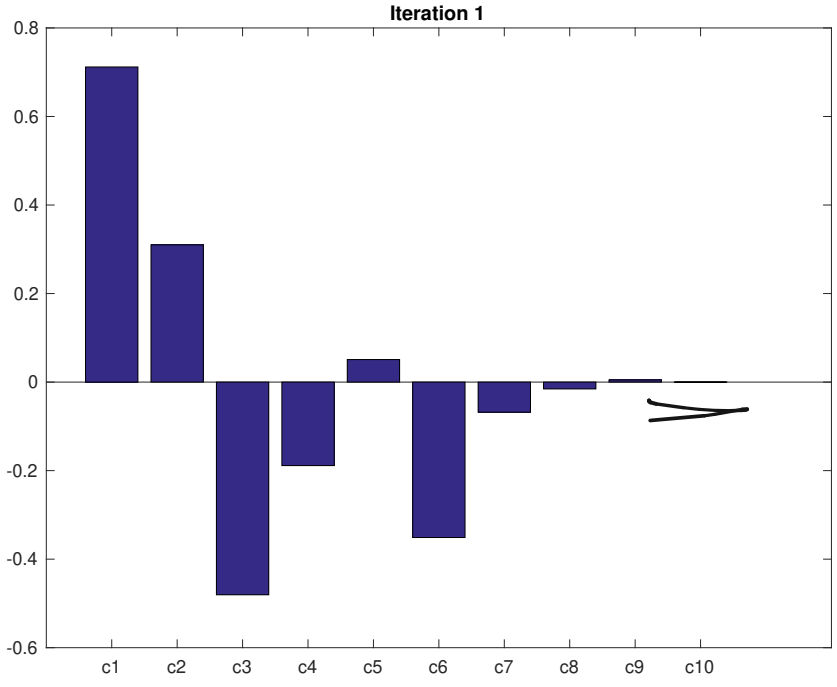

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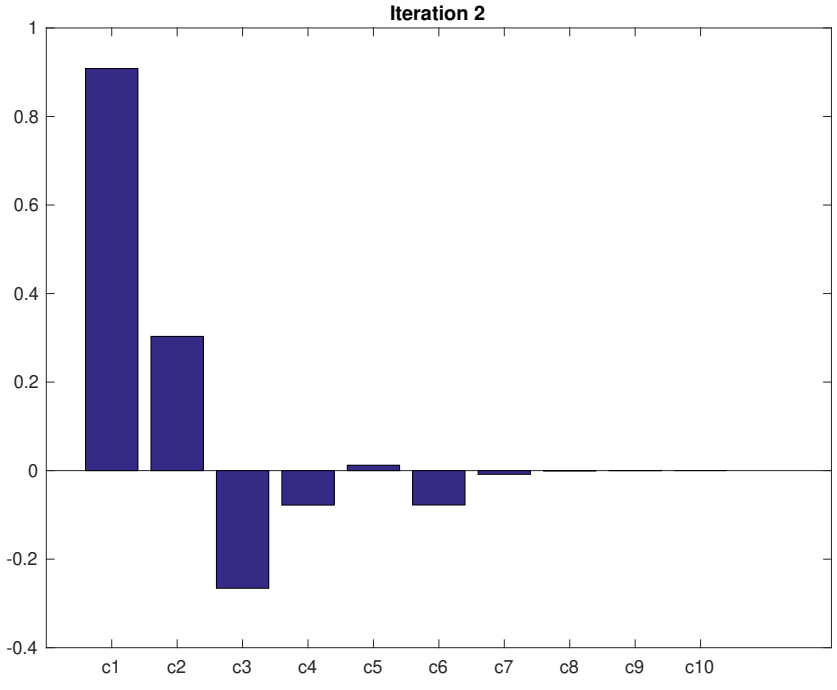

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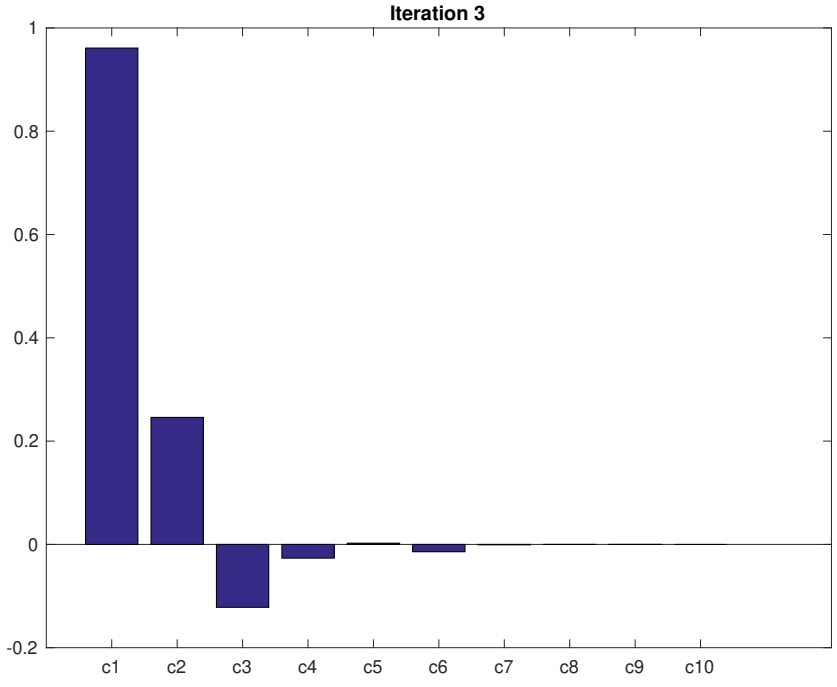

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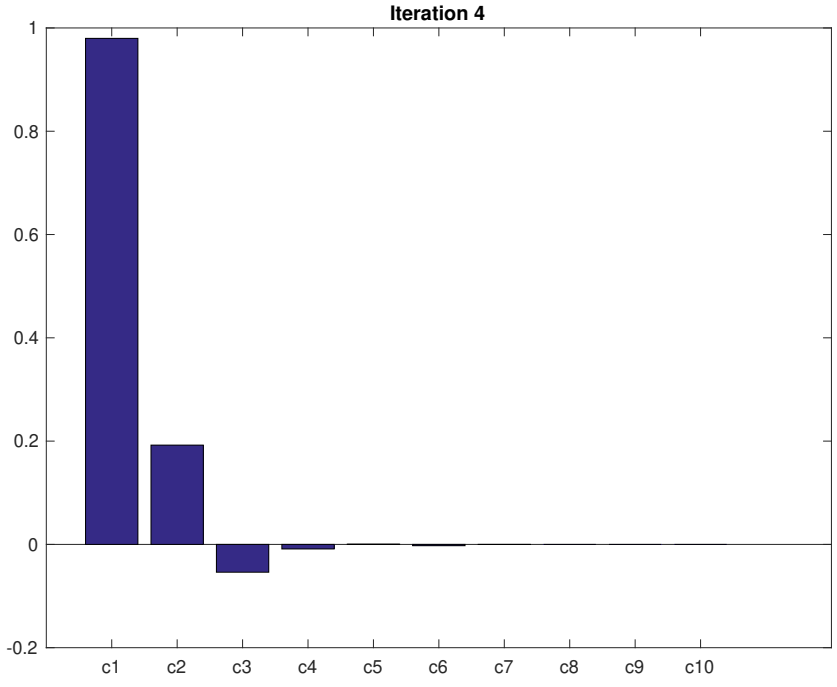

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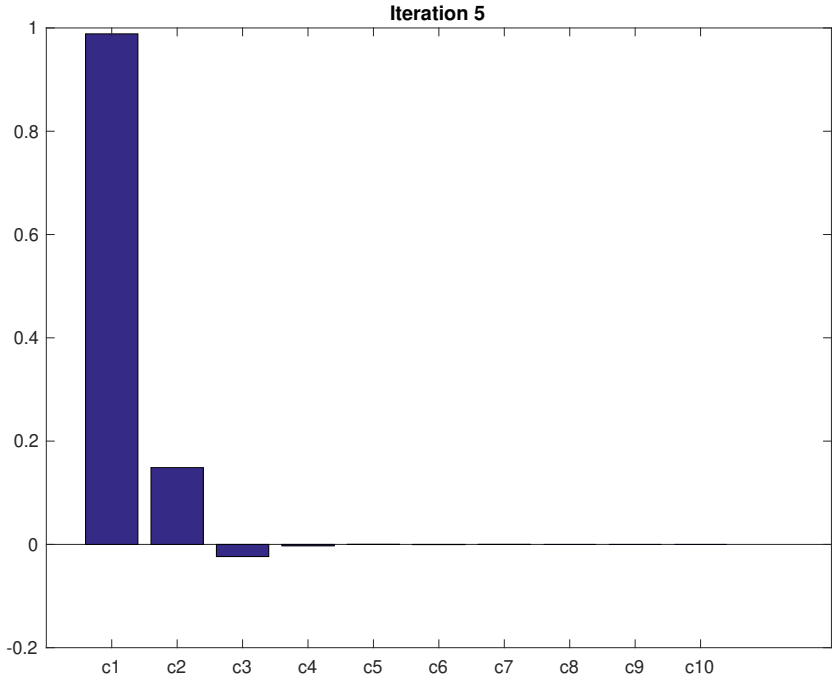

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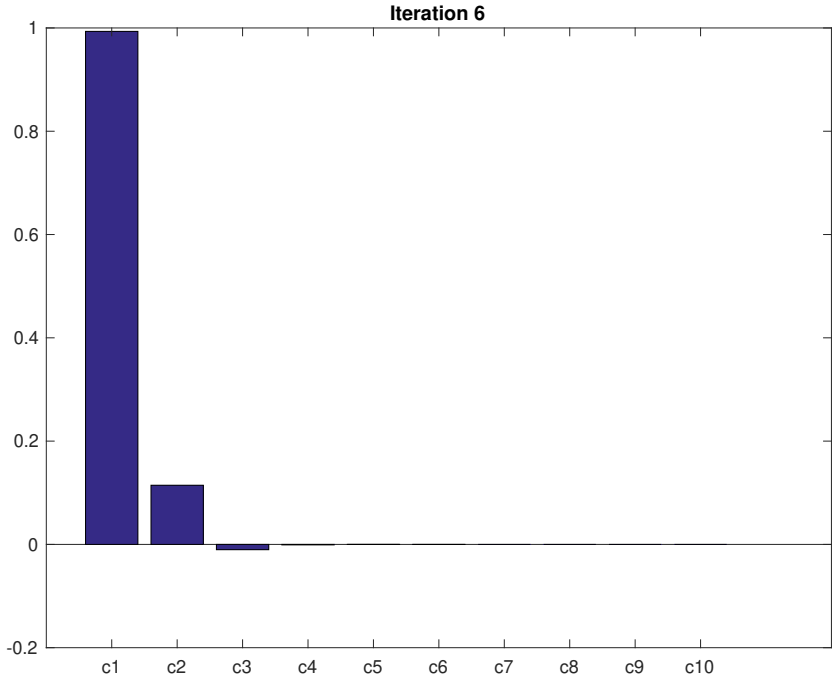

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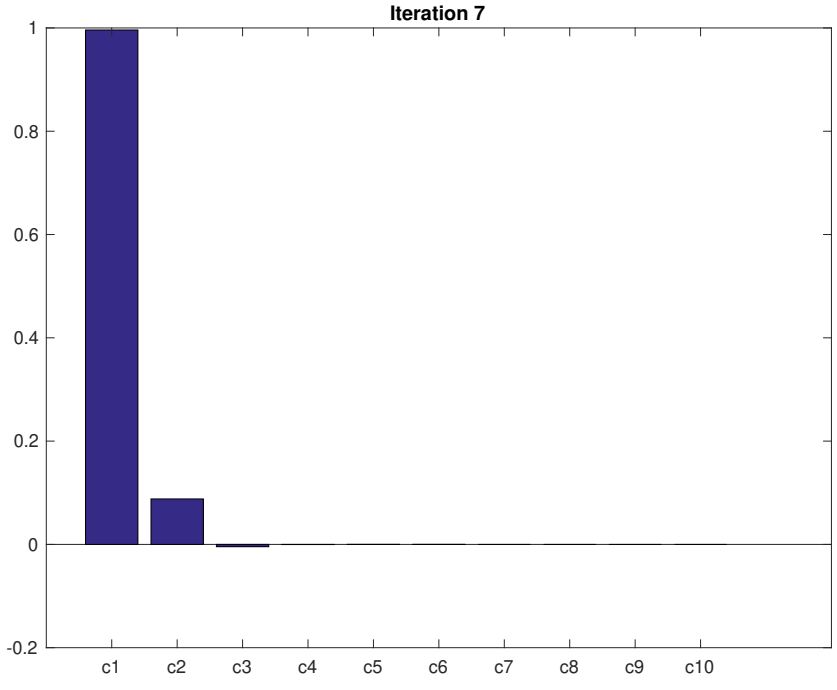

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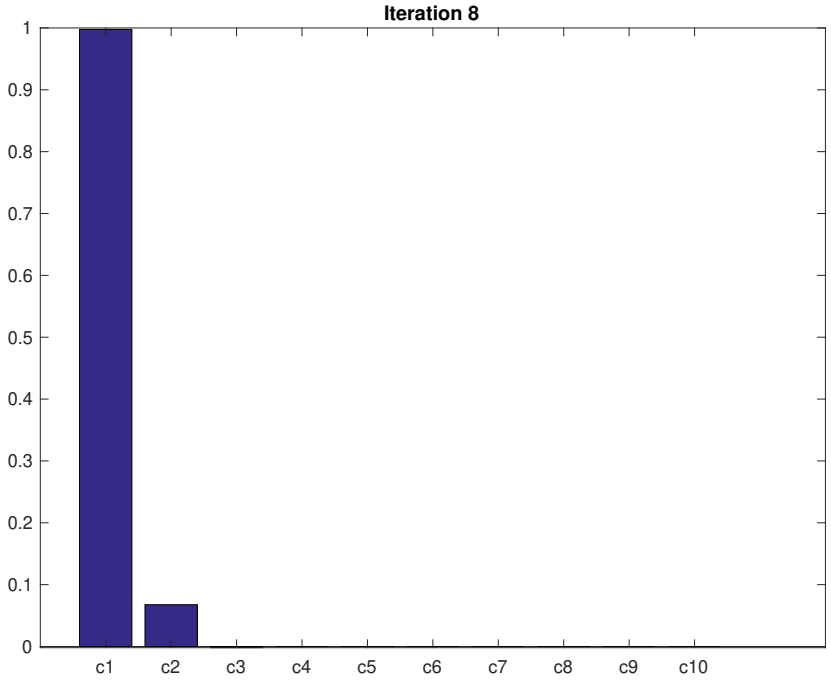

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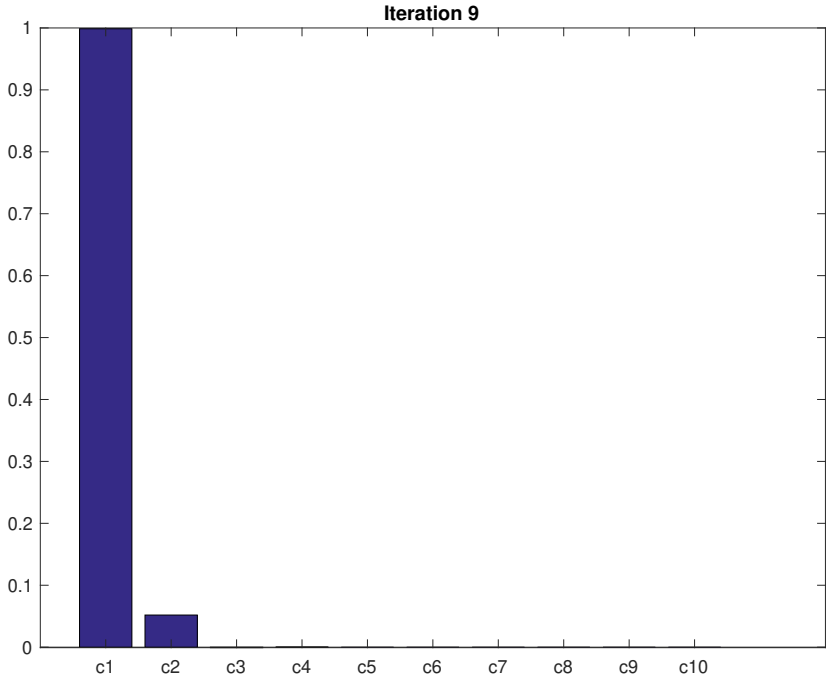

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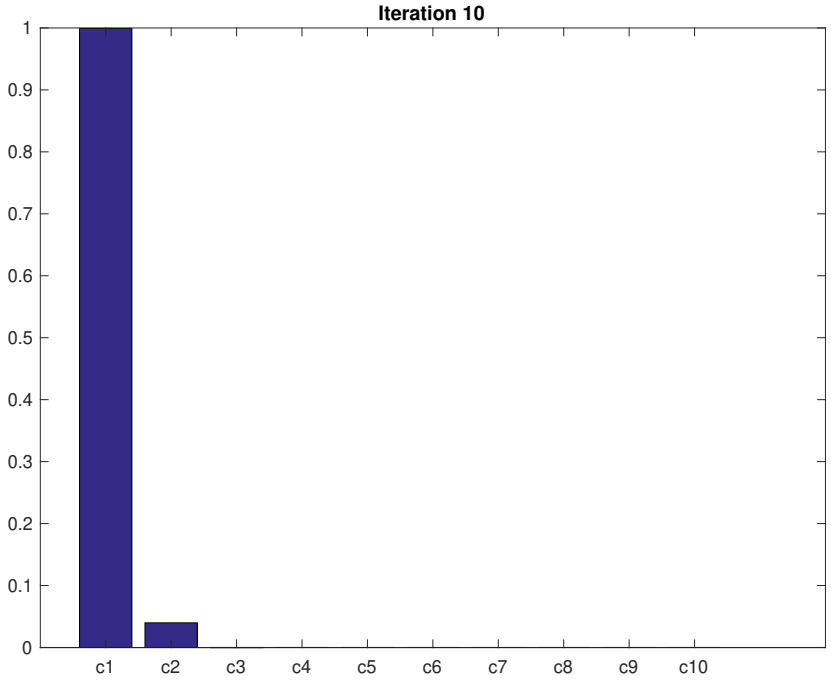

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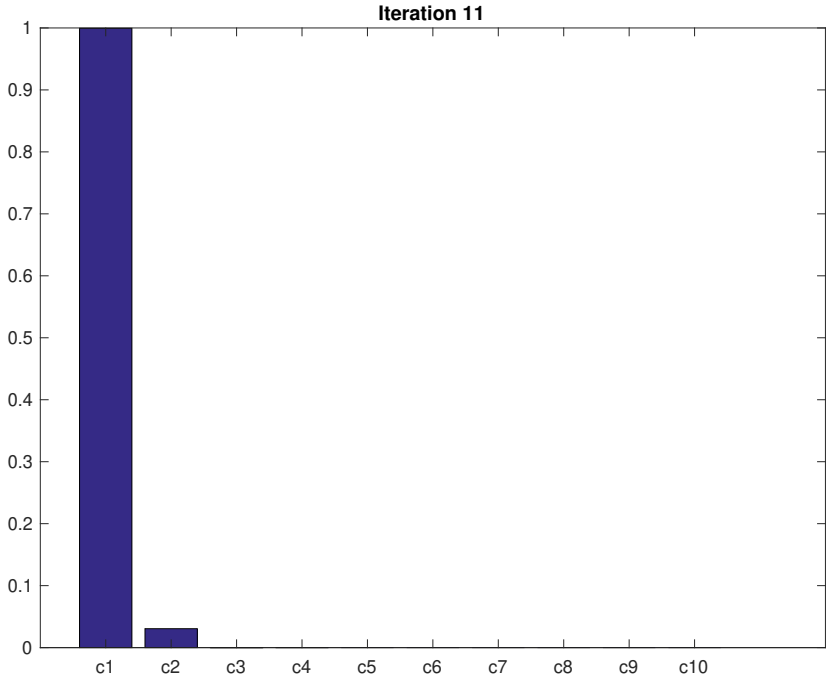

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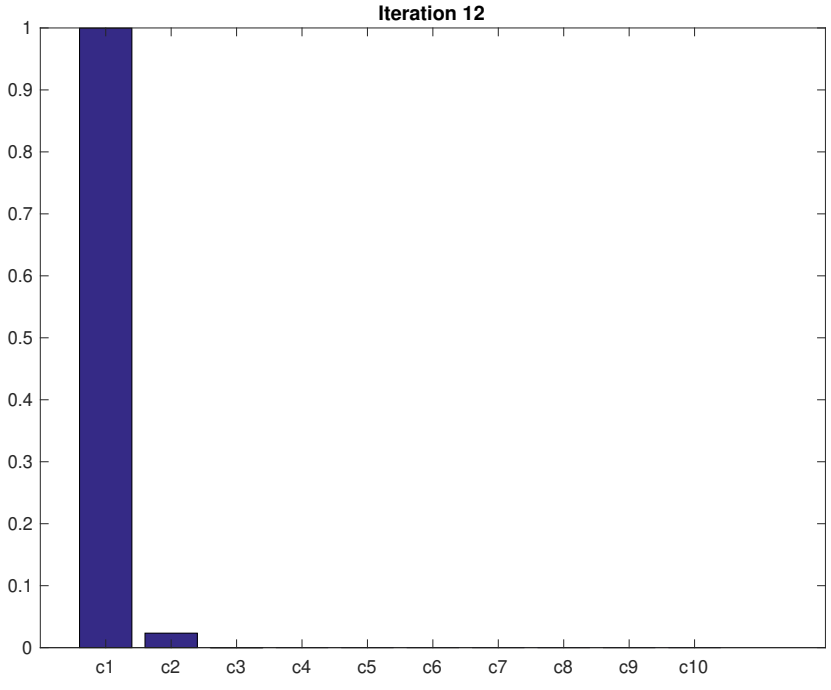

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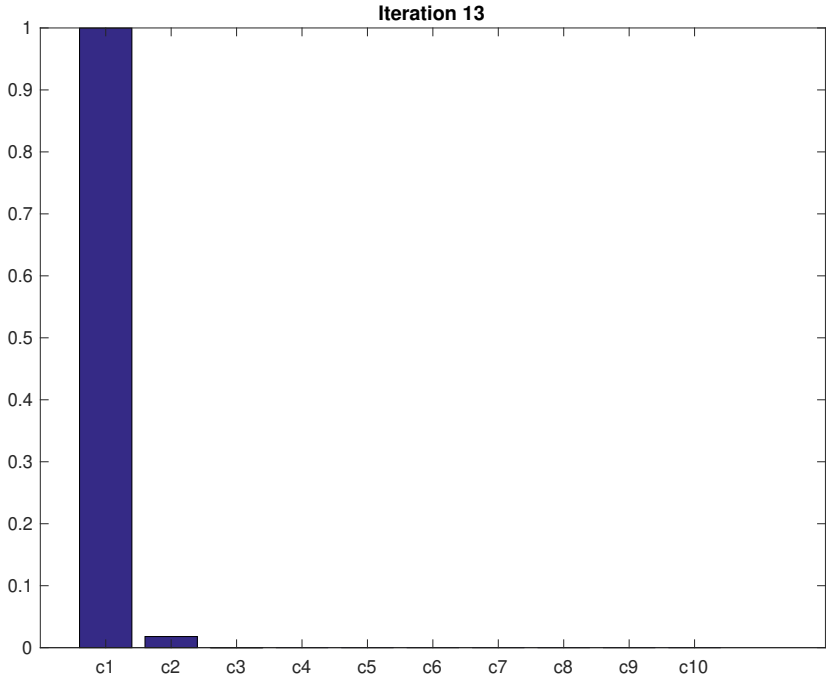

When will convergence be slow?

Power Method Slow Convergence

Slow Case: A has eigenvalues: $\lambda_1 = 1, \lambda_2 = .99, \lambda_3 = .9, \lambda_4 = .8, \ldots$

$$\vec{z}^{(0)} = c_1\vec{v}_1 + c_2\vec{v}_2 + \ldots + c_d\vec{v}_d \implies \vec{z}^{(t)} = c_1\lambda_1^t\vec{v}_1 + c_2\lambda_2^t\vec{v}_2 + \ldots + c_d\lambda_d^t\vec{v}_d$$

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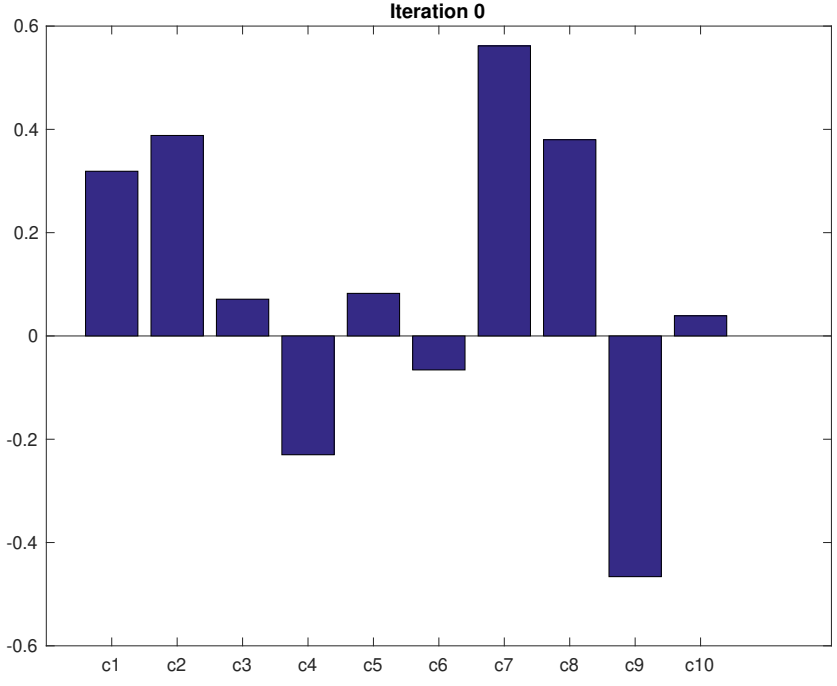

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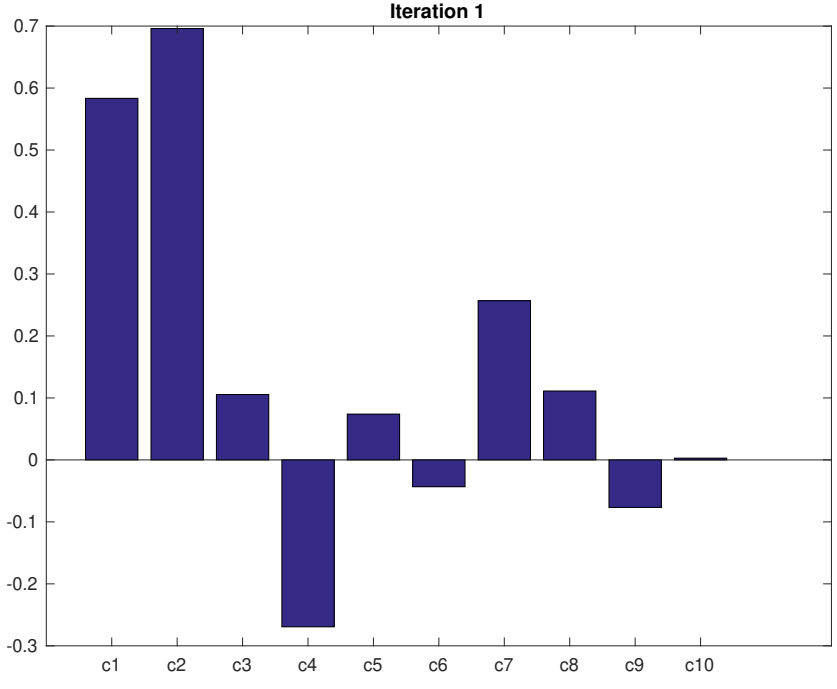

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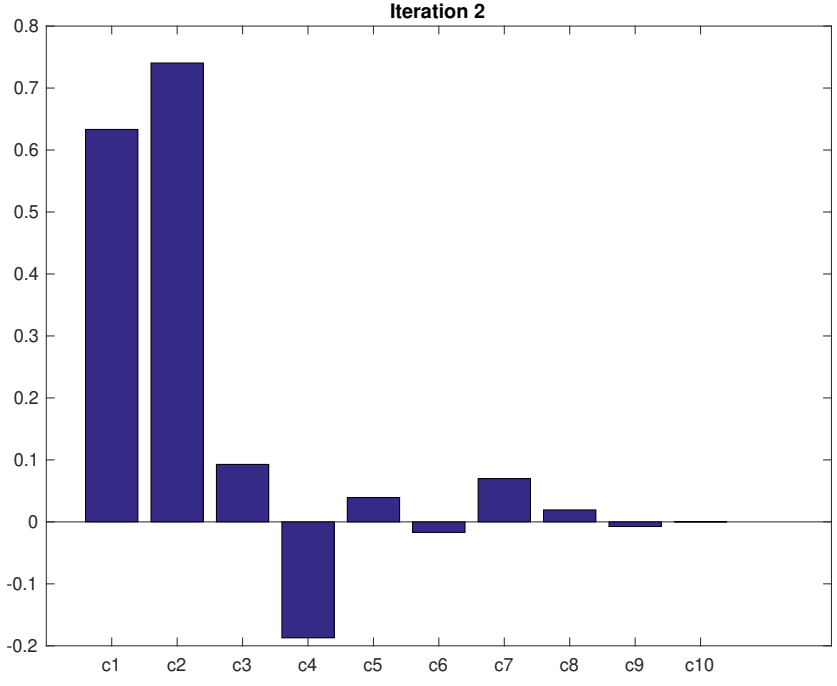

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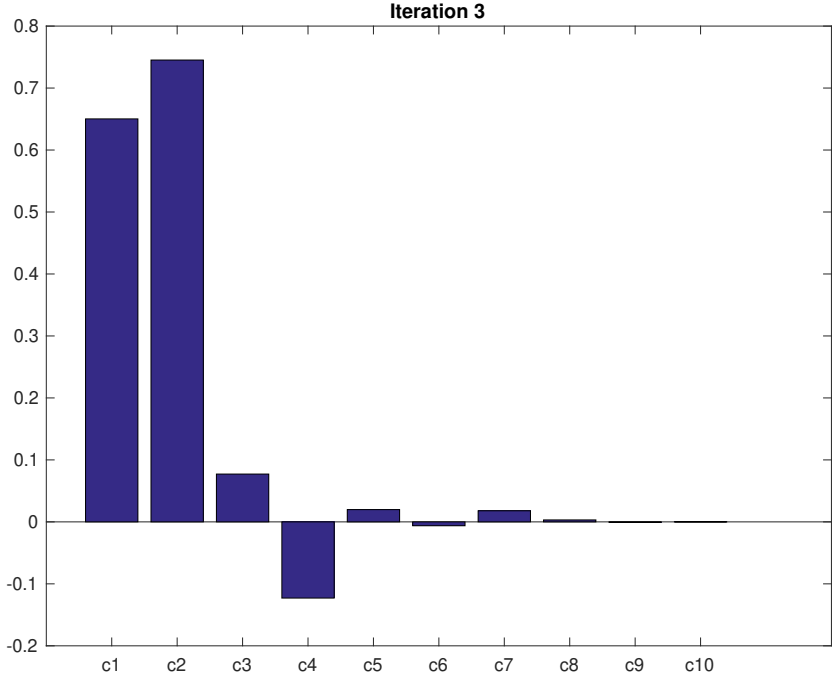

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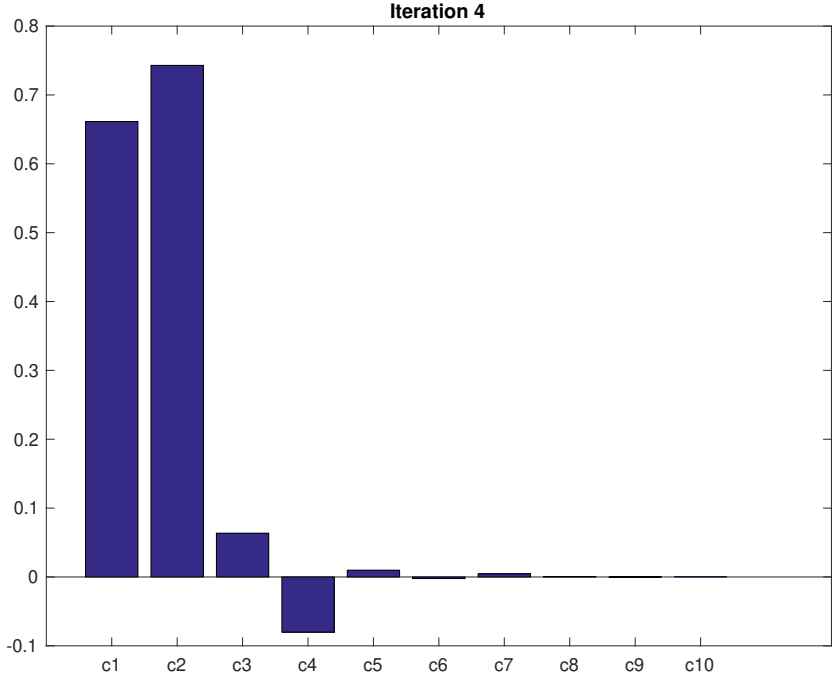

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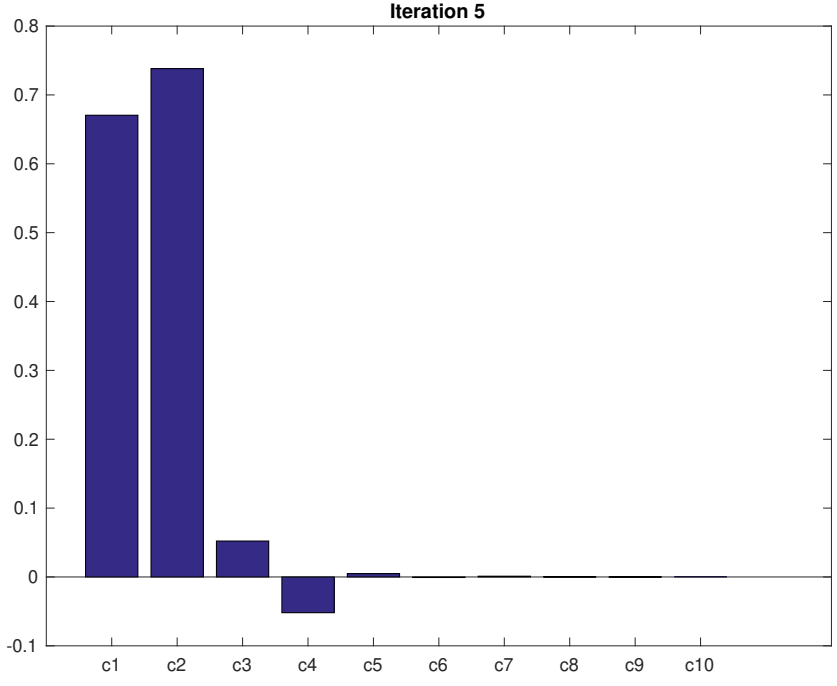

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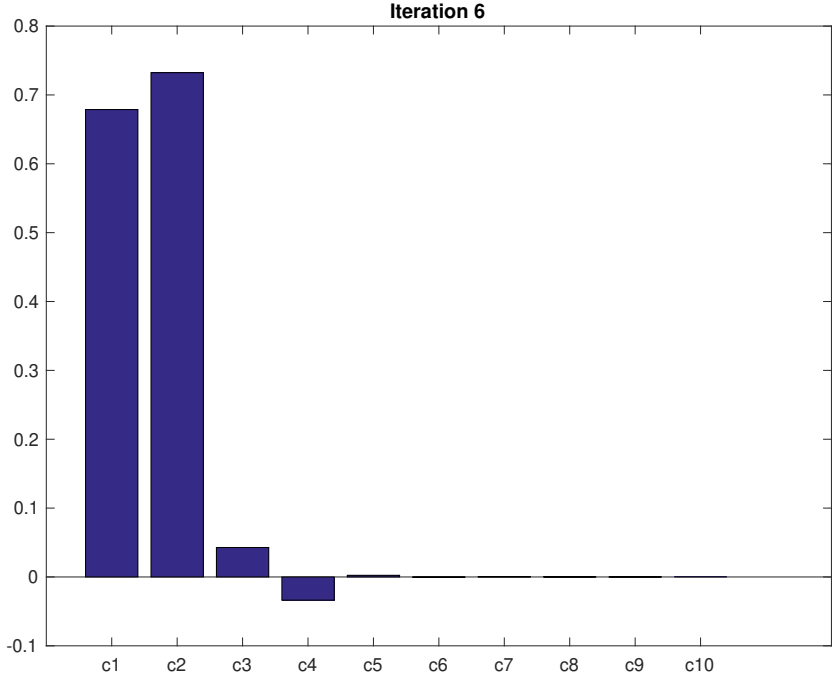

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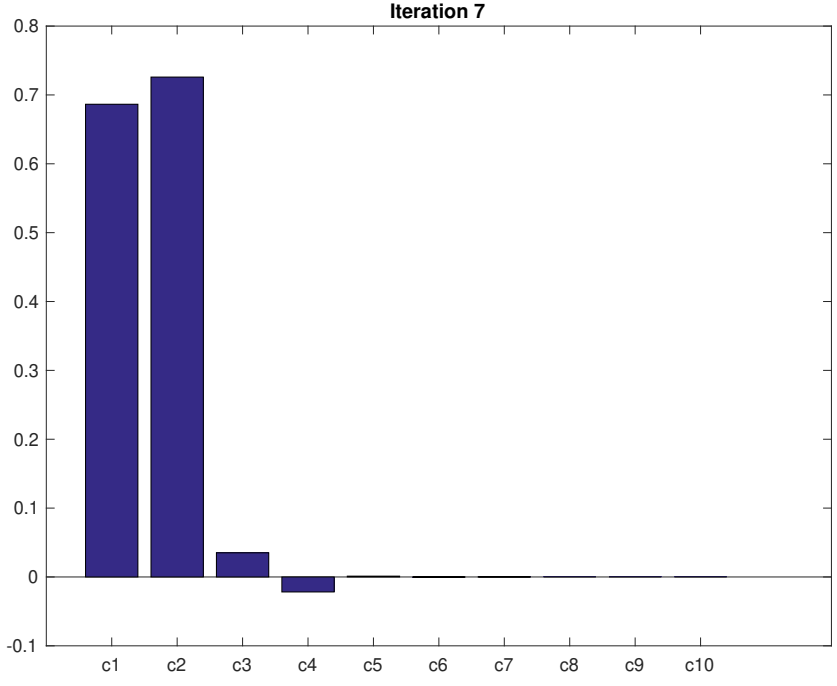

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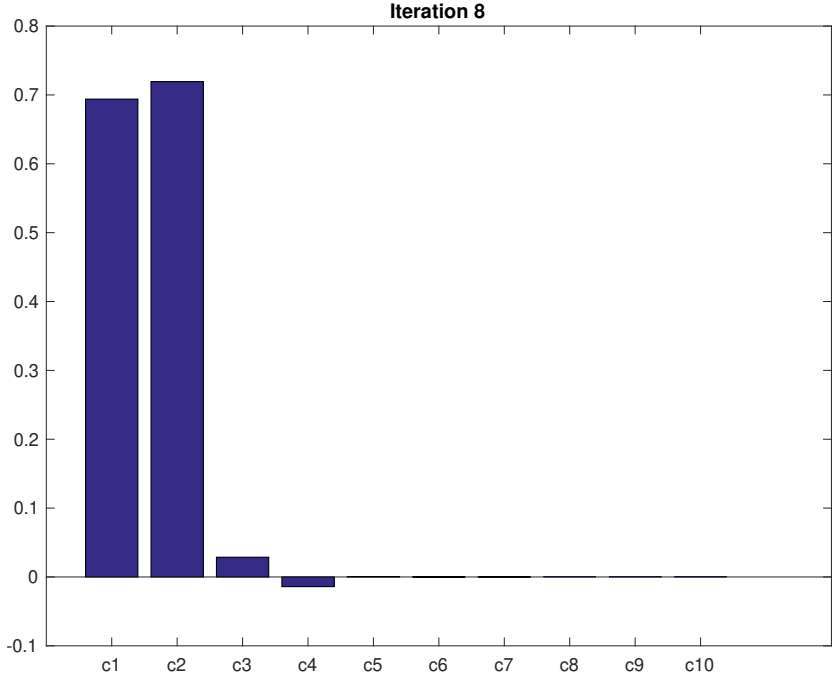

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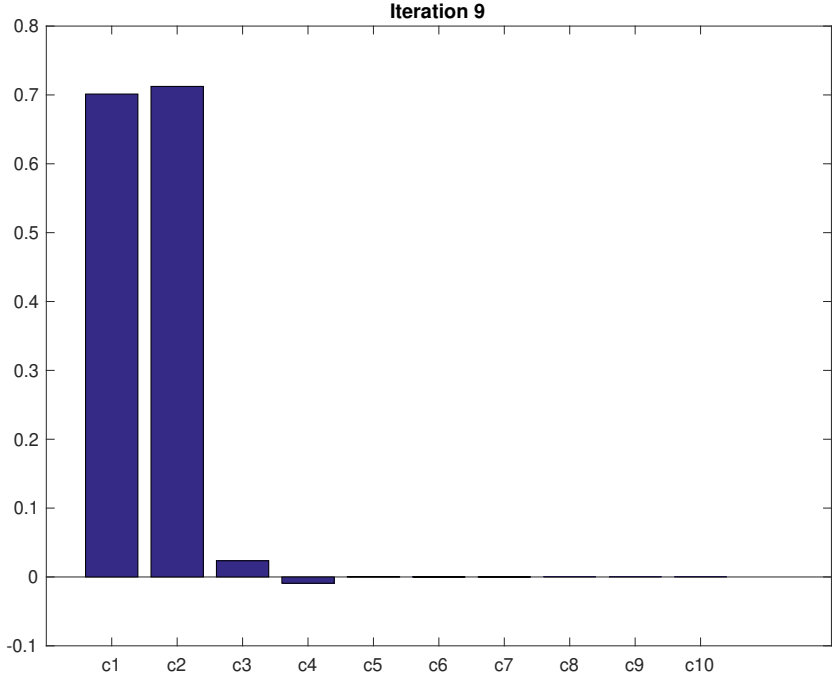

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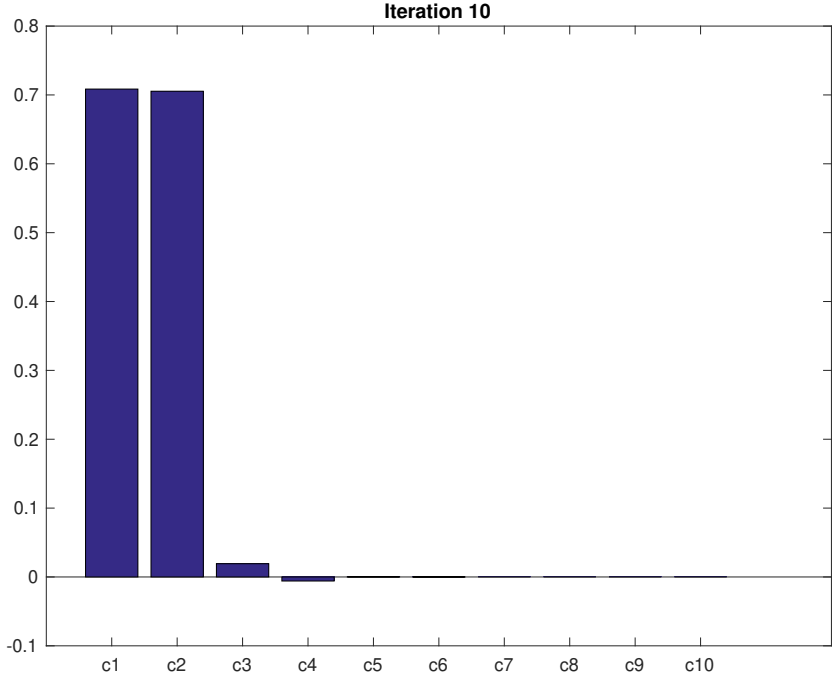

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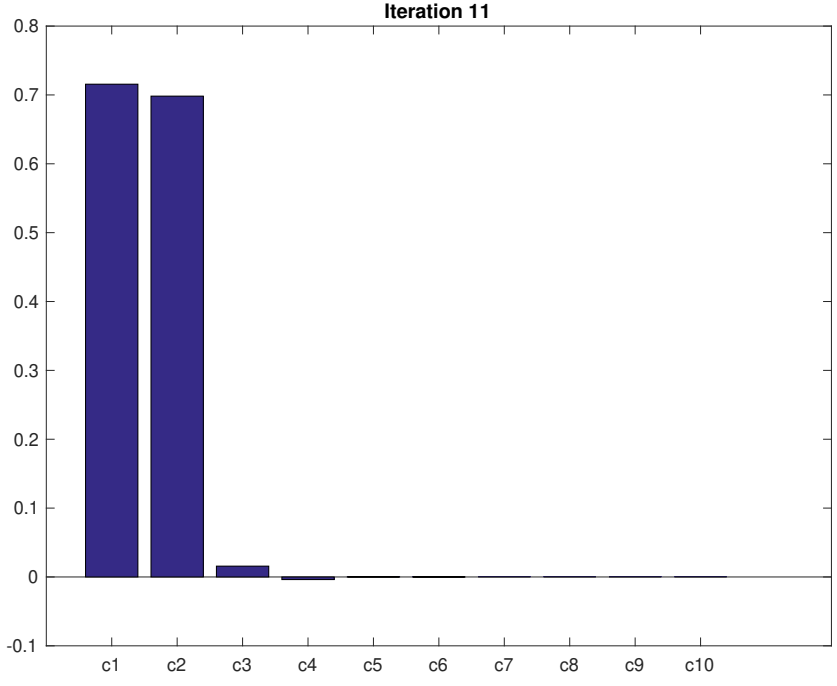

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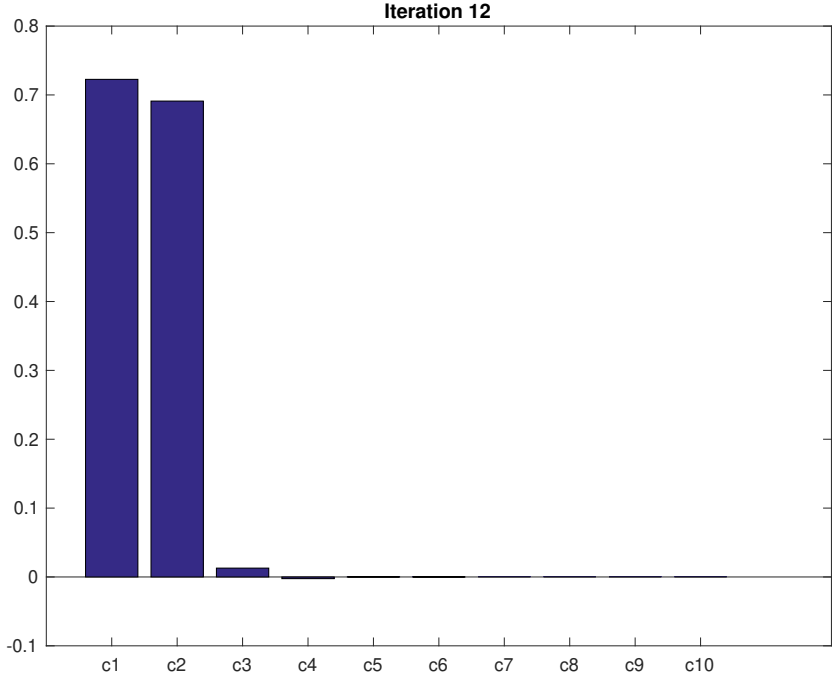

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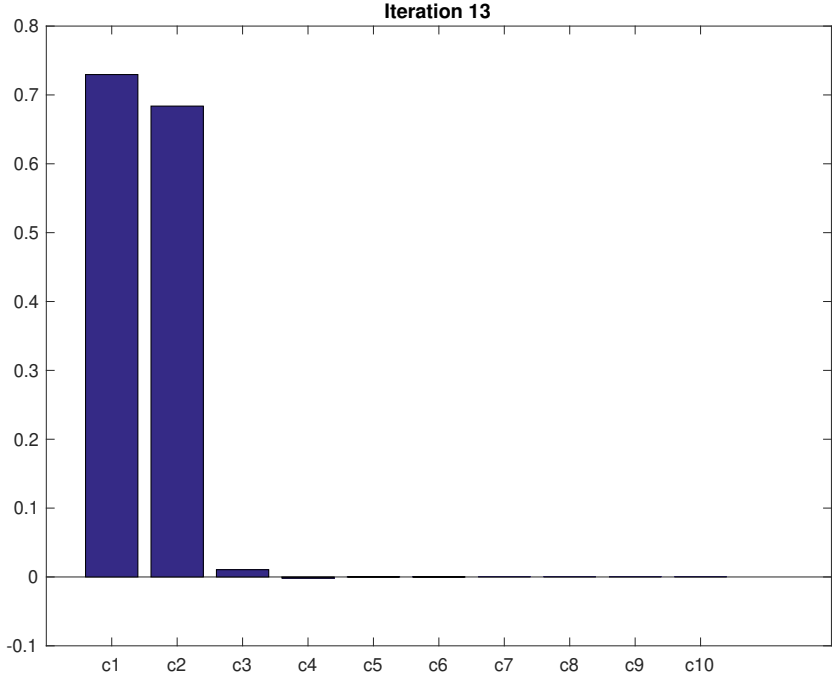

Power Method Convergence Rate

$$\vec{z}^{(0)} = c_1\vec{v}_1 + c_2\vec{v}_2 + \ldots + c_d\vec{v}_d \implies \vec{z}^{(t)} = c_1\lambda_1^t\vec{v}_1 + c_2\lambda_2^t\vec{v}_2 + \ldots + c_d\lambda_d^t\vec{v}_d$$

Write $|\lambda_2| = (1-\gamma)|\lambda_1|$ for 'gap' $\gamma = \frac{|\lambda_1| - |\lambda_2|}{|\lambda_1|}$.

How many iterations t does it take to have $|\lambda_2|^t \leq \frac{1}{e} \cdot |\lambda_1|^t$?

$$(1-\gamma)^t \lambda_1^t \leq \frac{1}{e} \lambda_1^t$$

$$(1-\gamma)^t \leq \frac{1}{e}$$

$$t = \log_{1-\gamma}\left(\frac{1}{e}\right) \approx O\left(\frac{1}{\gamma}\right)$$

$$(1-\gamma)^{1/\gamma} \approx \frac{1}{e}$$

$\mathbf{A} \in \mathbb{R}^{d\times d}$: input matrix with eigendecomposition $\mathbf{A} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^T$. $\vec{v}_1$: top eigenvector, being computed, $\vec{z}^{(i)}$: iterate at step i, converging to $\vec{v}_1$.

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How many iterations t does it take to have $|\lambda_2|^t \leq \delta \cdot |\lambda_1|^t$?

$\lambda_2^{1/\gamma \cdot m} \leq \frac{1}{e}\lambda_1^{1/\gamma \cdot m}$

$\lambda_2^{m/\gamma} \leq \frac{1}{e^m} \cdot \lambda_1^{m/\gamma}$

$e^m = \ln(1/\delta)$

$\frac{\ln(1/\delta)}{\gamma}$

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How small must we set δ to ensure that $c_1\lambda_1^t$ dominates all other components and so $\vec{z}^{(t)}$ is very close to $\vec{v}_1$?

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Random Initialization

Claim: When $z^{(0)}$ is chosen with random Gaussian entries, writing $z^{(0)} = c_1\vec{v}_1 + c_2\vec{v}_2 + \ldots + c_d\vec{v}_d$, with very high probability, for all i:

$$O(1/d^2) \leq |c_i| \leq O(\log d)$$

Corollary:

$$\max_j \left|\frac{c_j}{c_1}\right| \leq O(d^2 \log d).$$

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Claim 2: For gap $\gamma = \frac{|\lambda_1| - |\lambda_2|}{|\lambda_1|}$, and $t = \frac{\ln(1/\delta)}{\gamma}$, $\left|\frac{\lambda_i^t}{\lambda_1^t}\right| \leq \delta$ for all i.

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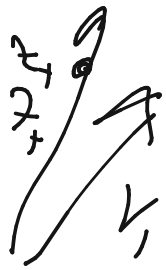
$$\|\vec{z}^{(t)} - \vec{v}_1\|_2 \leq \left\| \frac{c_1\lambda_1^t\vec{v}_1 + \ldots + c_d\lambda_d^t\vec{v}_d}{\|c_1\lambda_1^t\vec{v}_1\|_2} - \vec{v}_1 \right\|_2$$



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$\mathbf{A} \in \mathbb{R}^{d\times d}$: input matrix with eigendecomposition $\mathbf{A} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^T$. $\vec{v}_1$: top eigenvector, being computed, $\vec{z}^{(i)}$: iterate at step i, converging to $\vec{v}_1$.

Random Initialization

Claim 1: When $z^{(0)}$ is chosen with random Gaussian entries, writing $z^{(0)} = c_1\vec{v}_1 + c_2\vec{v}_2 + \ldots + c_d\vec{v}_d$, with very high probability, $\max_j \left|\frac{c_j}{c_1}\right| \leq O(d^2 \log d)$.

Claim 2: For gap $\gamma = \frac{|\lambda_1|-|\lambda_2|}{|\lambda_1|}$, and $t = \frac{\ln(1/\delta)}{\gamma}$, $\left|\frac{\lambda_i^t}{\lambda_1^t}\right| \leq \delta$ for all i.

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Setting $\delta = O\left(\frac{\epsilon}{d^3 \log d}\right)$ gives $\|\vec{z}^{(t)} - \vec{v}_1\|_2 \leq \epsilon$.

$\log(1/\delta) \sim O(\log(d/\epsilon))$

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Power Method Theorem

Theorem (Basic Power Method Convergence)
Let $\gamma = \frac{|\lambda_1| - |\lambda_2|}{|\lambda_1|}$ be the relative gap between the first and second eigenvalues. If Power Method is initialized with a random Gaussian vector $\vec{v}^{(0)}$ then, with high probability, after $t = O\left(\frac{\ln(d/\epsilon)}{\gamma}\right)$ steps:

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krylov subspace methods

Krylov subspace methods (Lanczos method, Arnoldi method.)

- How `svds`/`eigs` are actually implemented. Only need $t = O\left(\frac{\ln(d/\epsilon)}{\sqrt{\gamma}}\right)$ steps for the same guarantee.

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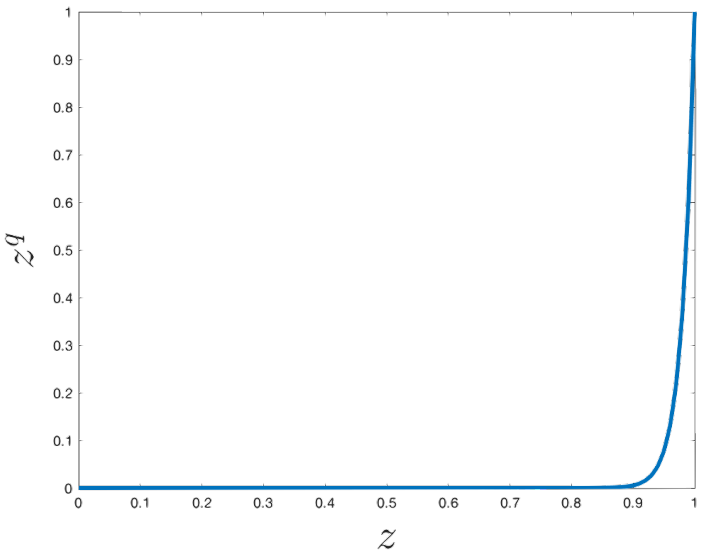
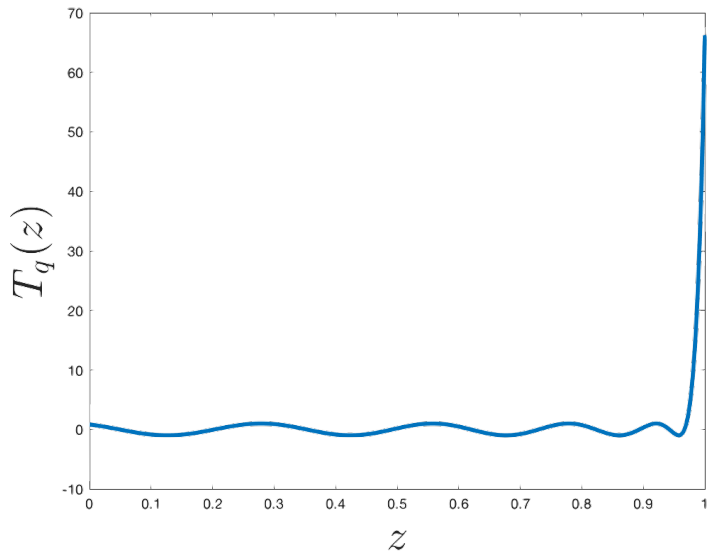
- Still requires just t matrix vector multiplies. Why?

krylov subspace methods



VS.



generalizations to larger k

- Block Power Method (a.k.a. Simultaneous Iteration, Subspace Iteration, or Orthogonal Iteration)
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$$\text{Runtime: } O\left(ndk \cdot \frac{\ln(d/\epsilon)}{\sqrt{\gamma}}\right)$$

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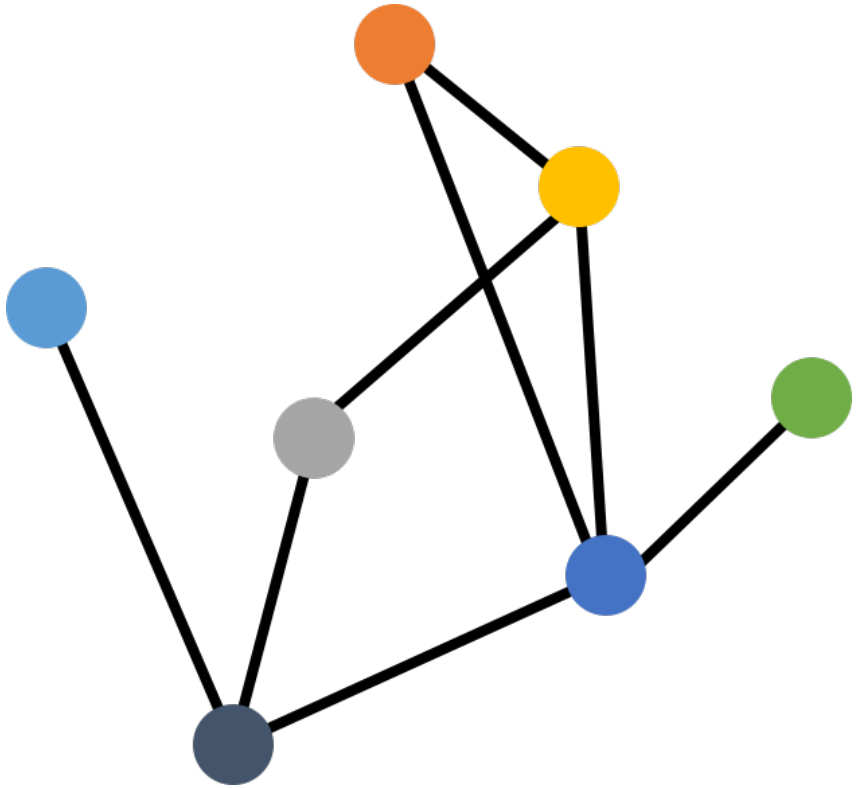
$$\text{'Gapless' Runtime: } O\left(ndk \cdot \frac{\ln(d/\epsilon)}{\sqrt{\epsilon}}\right)$$

if you just want a set of vectors that gives an ϵ-optimal low-rank approximation when you project onto them.

Connection Between Random Walks, Eigenvectors, and Power Method (Bonus Material)

Connection to Random Walks

Consider a random walk on a graph G with adjacency matrix $\mathbf{A}$.



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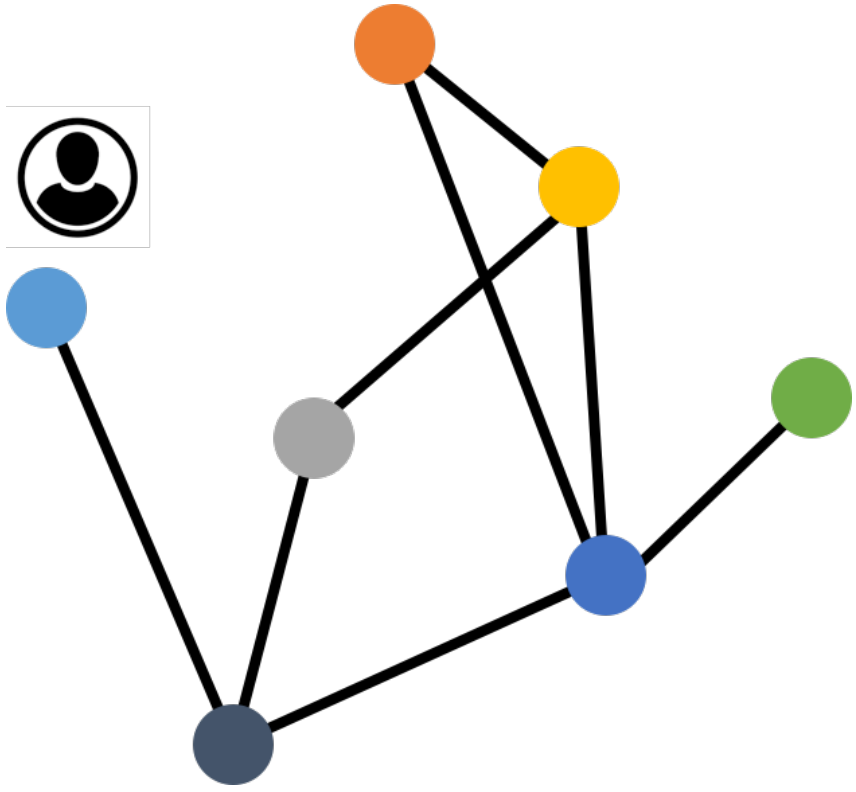

At each step, move to a random vertex, chosen uniformly at random from the neighbors of the current vertex.

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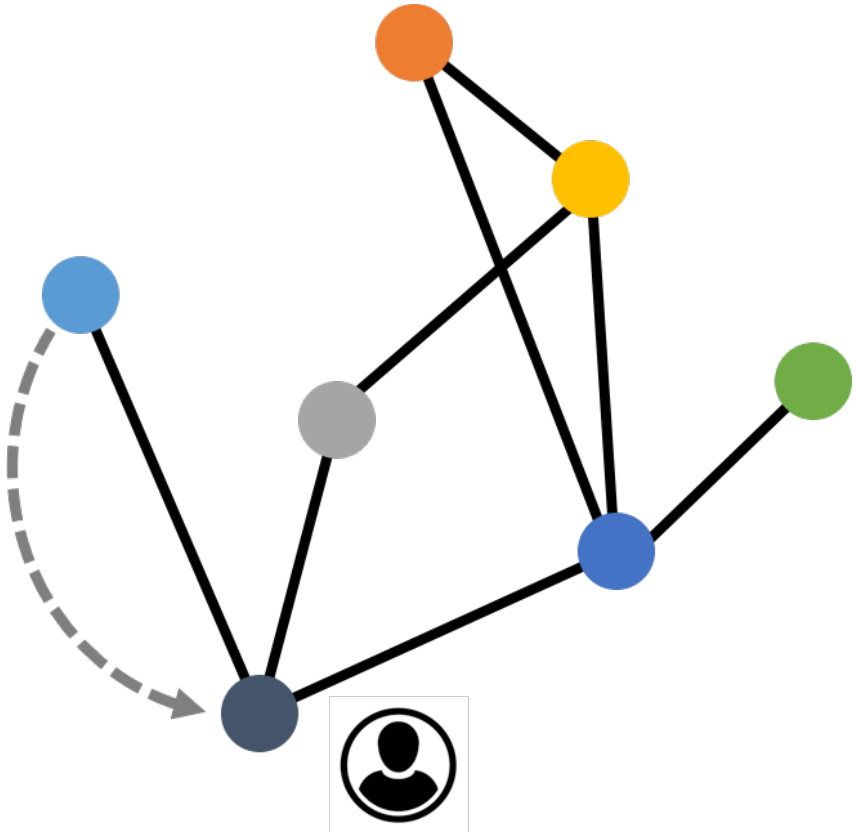

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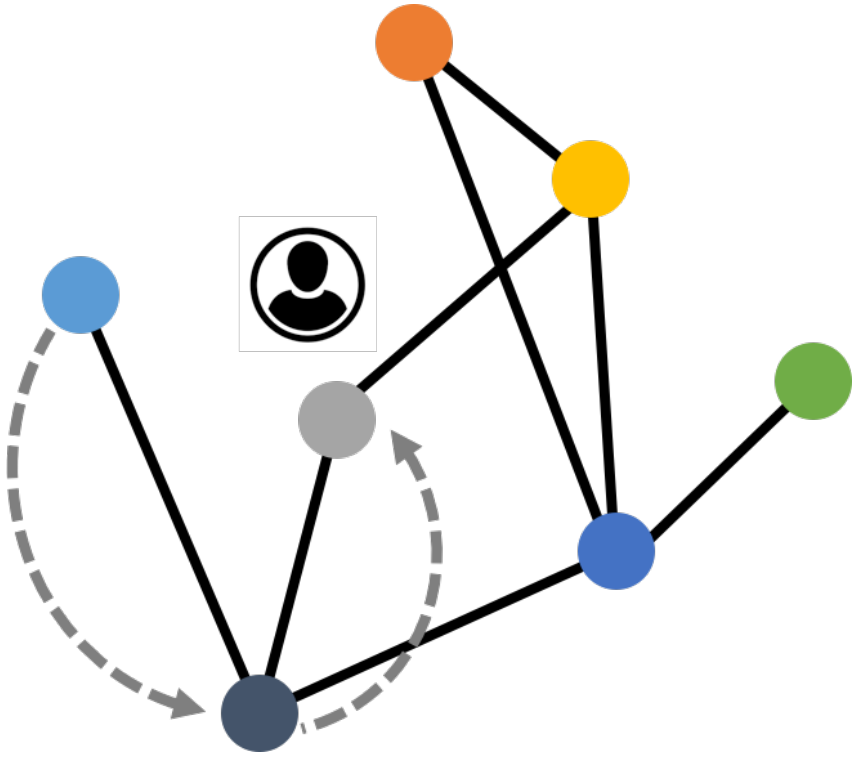

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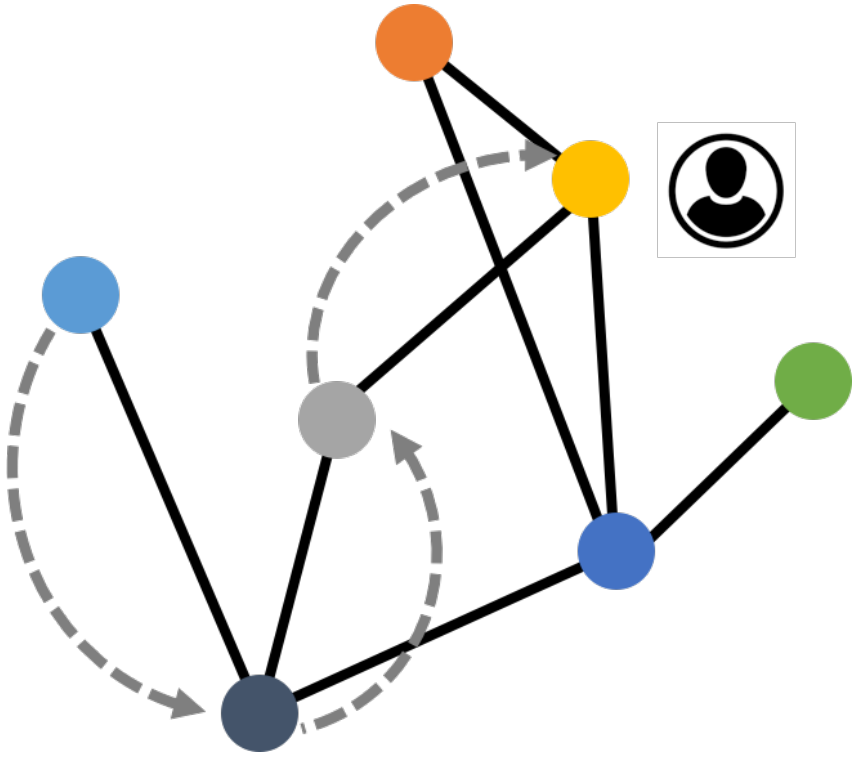

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Claim: After t steps, the probability that a random walk is at node i is given by the i^{th} entry of

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- Like the power method, the time a random walk takes to converge to its stationary distribution (mixing time) is dependent on the gap between the top two eigenvalues of $\mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2}$. The spectral gap.