COMPSCI 514: Algorithms for Data Science

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University of Massachusetts Amherst. Spring 2026.

Lecture 18

Logistics

- Midterm **in class next Thursday 4/23**.
- See Piazza/last lecture/midterm study guide for details.
- Will cover material up to this lecture.
- The quiz this week is **optional**. If you take it, it will replace your second lowest regular quiz grade (the lowest is dropped).

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. Quick sketch of 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 modern data science/ML.

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 and graphs.

How efficient are these techniques? Can they be run on very 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 approximation 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 $O(nd^2)$.

$k << d$

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

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 $\mathbf{A}$.

$A v_1 = \lambda_1$

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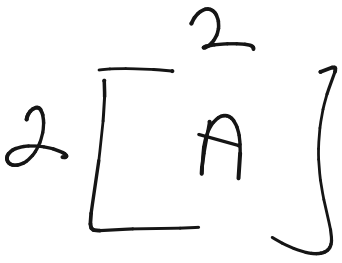
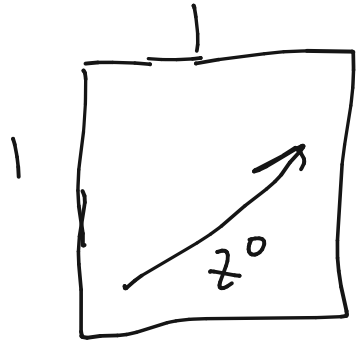
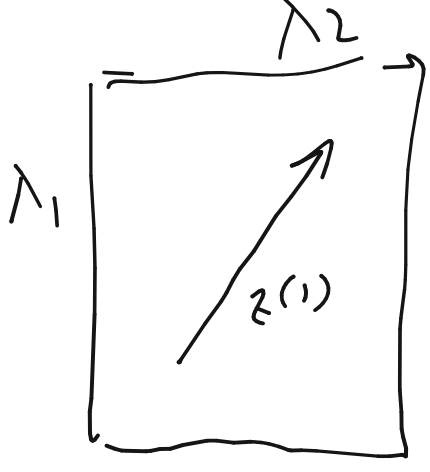
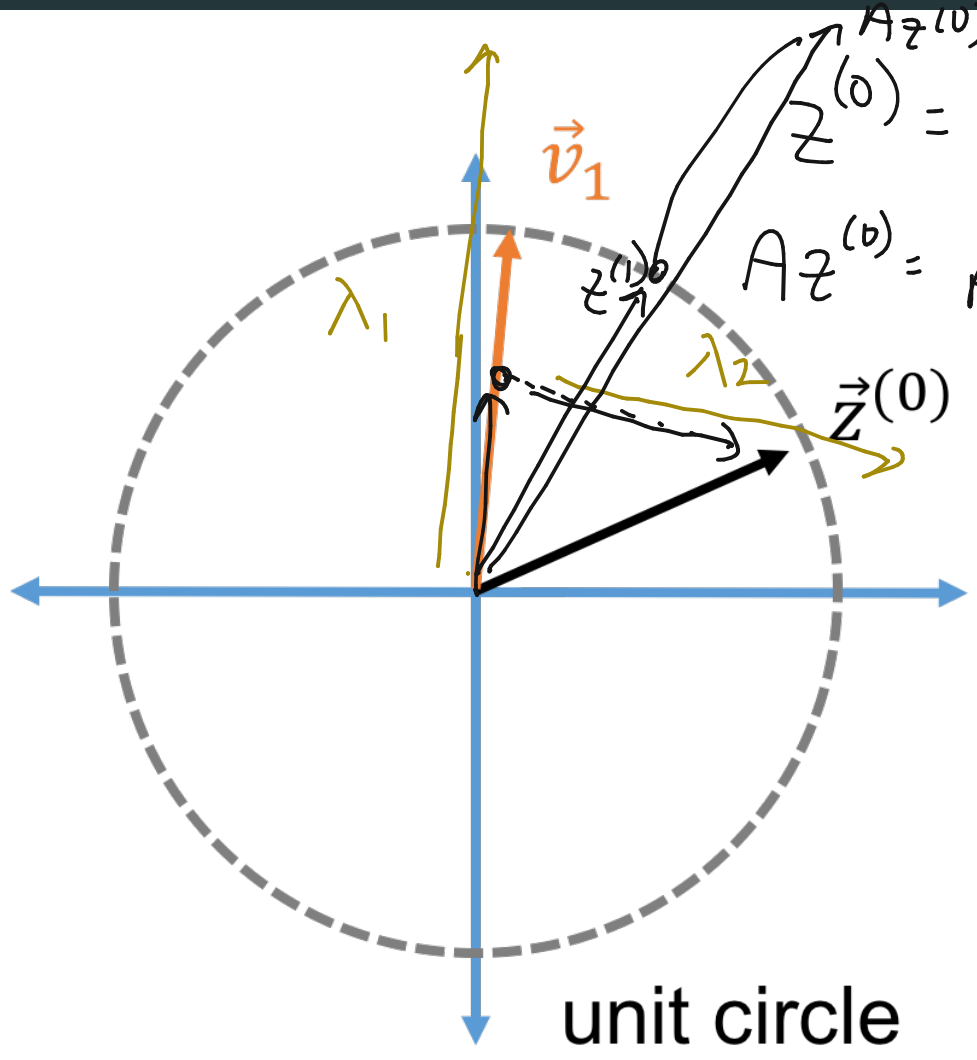
- **Initialize:** Choose $\vec{z}^{(0)}$ randomly. E.g. $\vec{z}^{(0)}(i) \sim \mathcal{N}(0, 1)$.
- For $i = 1, \ldots, t$
  - $\vec{z}^{(i)} := \mathbf{A} \cdot \vec{z}^{(i-1)}$
  - $\vec{z}^{(i)} := \frac{\vec{z}^{(i)}}{\|\vec{z}^{(i)}\|_2}$ (unit vector)
- Return $\vec{z}^{(t)}$

Power Method







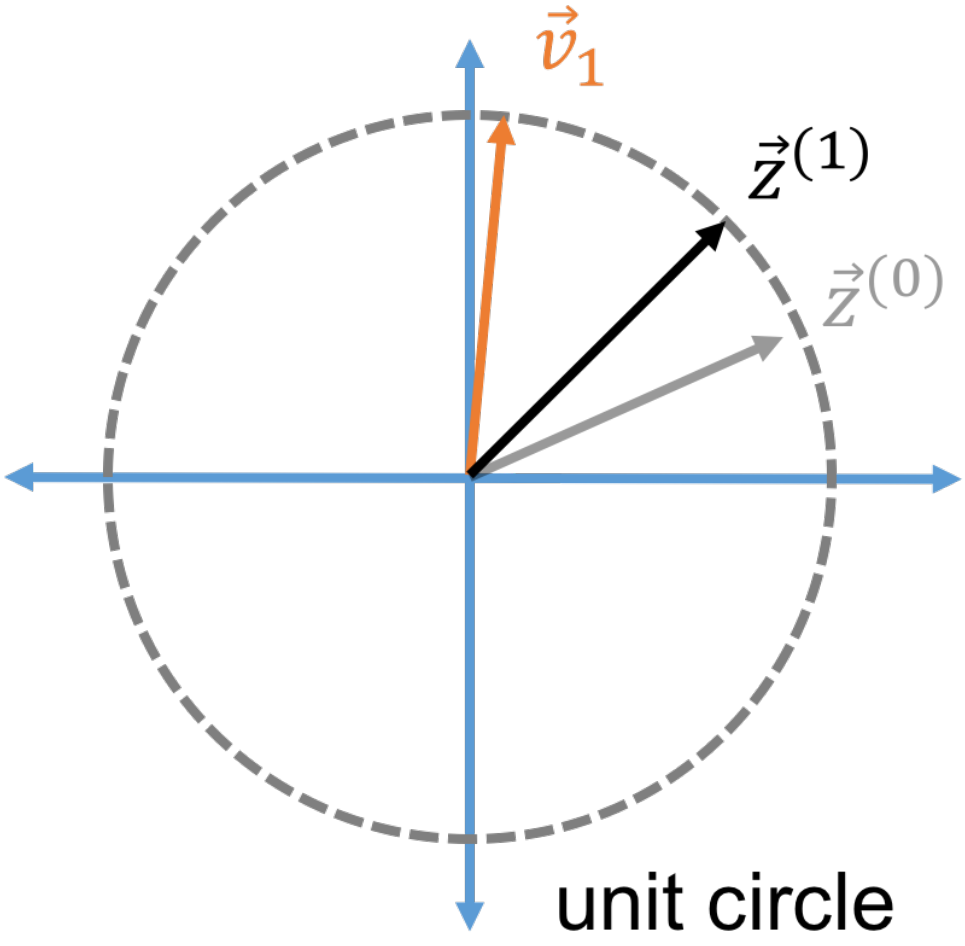


$$z^{(0)} = c_1 v_1 + c_2 v_2$$

$$Az^{(0)} = A(c_1 v_1) + A(c_2 v_2)$$

$$\lambda_2 < \lambda_1$$

Power Method



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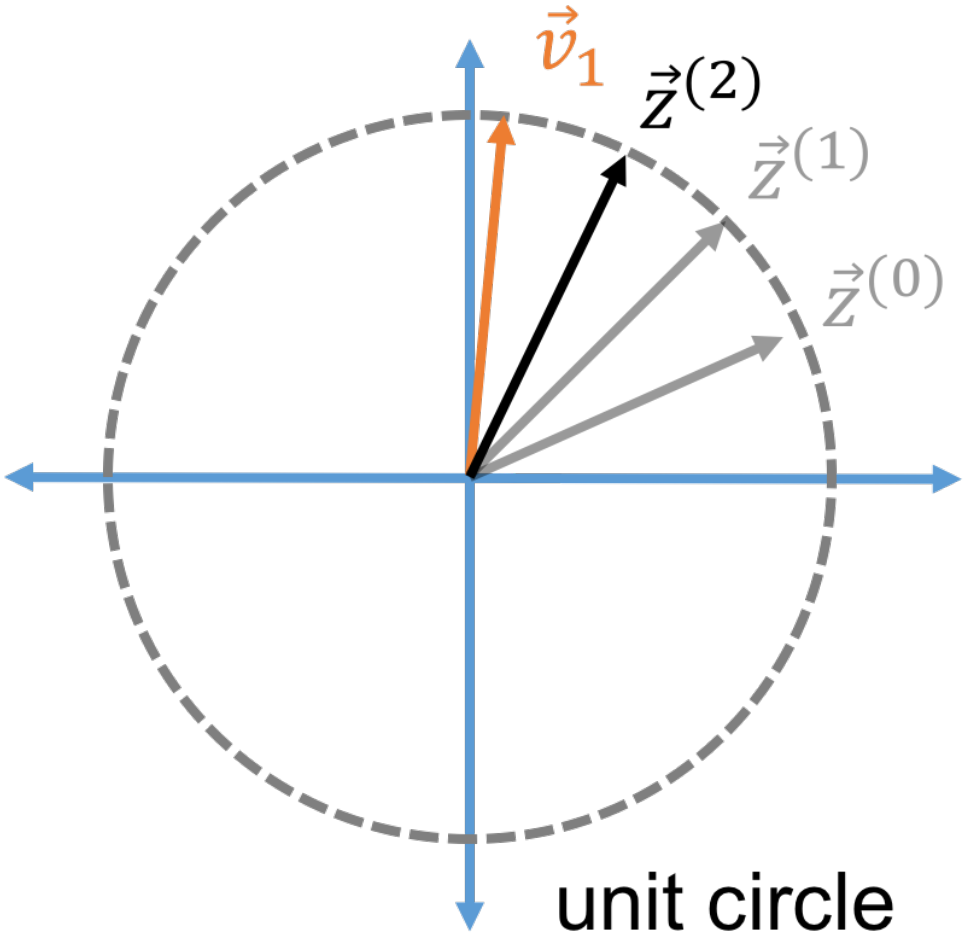

Power Method Analysis

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Theoretically equivalent to:

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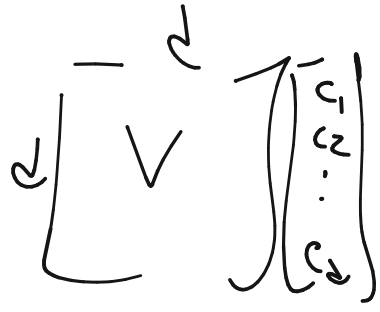
Power Method Analysis

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

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



$\mathbf{A} \in \mathbb{R}^{d\times d}$: 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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Az

$(V(\Lambda(V^T z)))$

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)

1. $\mathbf{V}^T\vec{z}^{(0)} = V^T V c = c = \begin{bmatrix} c_1 \\ \vdots \\ c_d \end{bmatrix}$

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

3. $\vec{z}^{(1)} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^T \cdot \vec{z}^{(0)} = \begin{bmatrix} V \end{bmatrix}\begin{bmatrix} \lambda_1 c_1 \\ \vdots \\ \lambda_d c_d \end{bmatrix} = V_1 \cdot \lambda_1 c_1 + V_2 \lambda_2 c_2 + \ldots + V_d \cdot \lambda_d c_d$

$\mathbf{A} \in \mathbb{R}^{d\times d}$: 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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Claim 1 : Writing $\vec{z}^{(0)} = c_1\vec{v}_1 + c_2\vec{v}_2 + \ldots + c_d\vec{v}_d$,

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$$\vec{z}^{(2)} = \mathbf{A}\vec{z}^{(1)} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^T\vec{z}^{(1)} = c_1\lambda_1^2\vec{v}_1 + \ldots + c_d\lambda_d^2\vec{v}_d$$

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Claim 2:

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

huge

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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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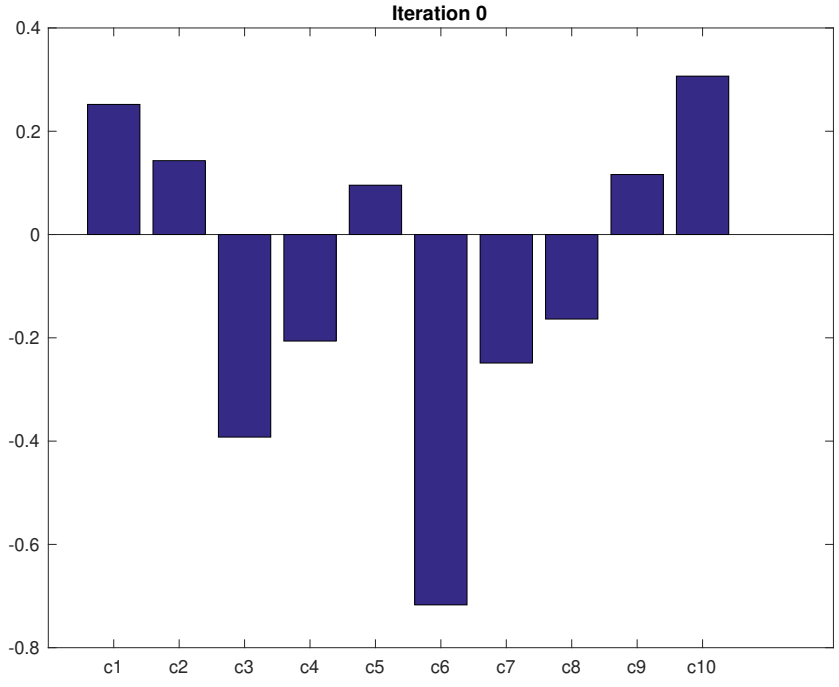

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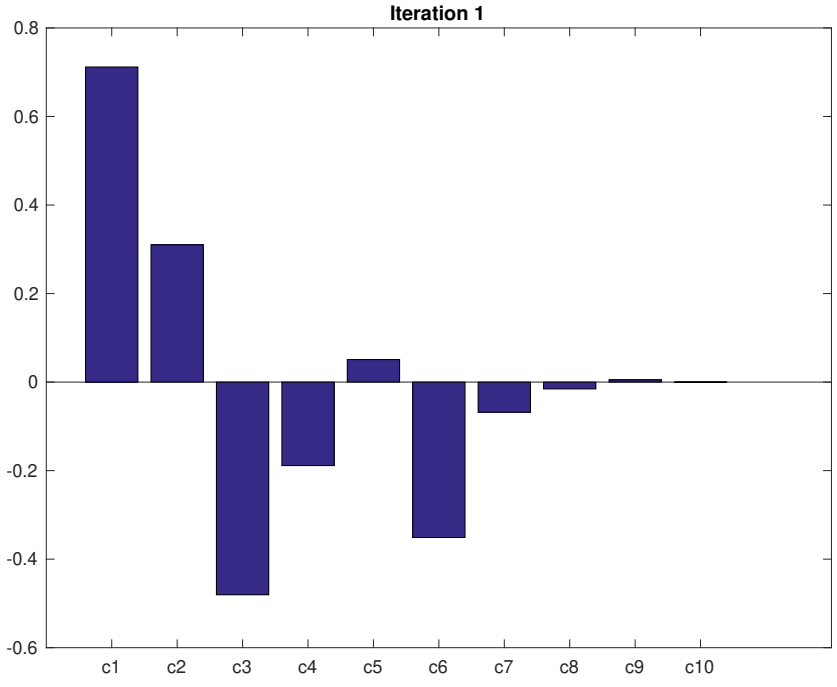

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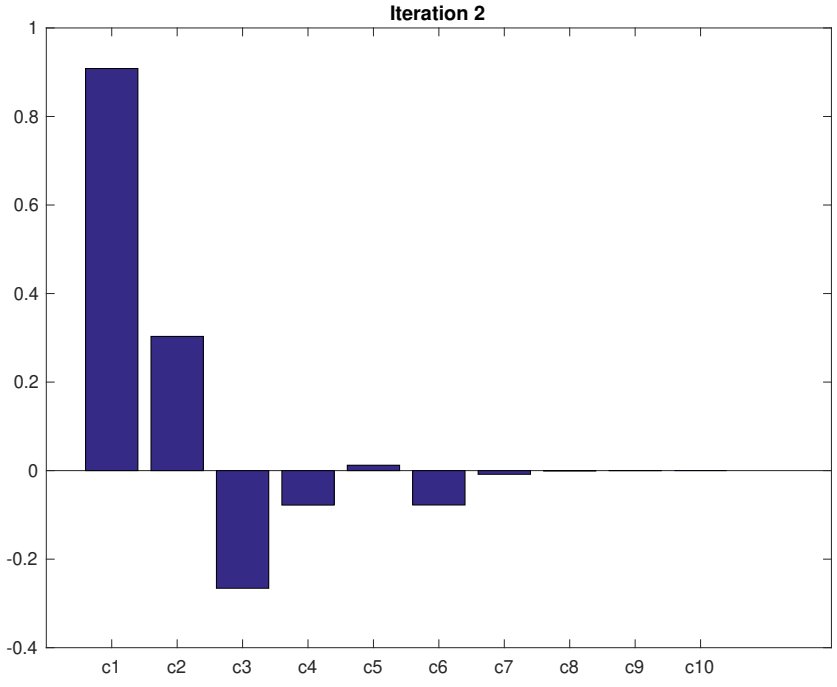

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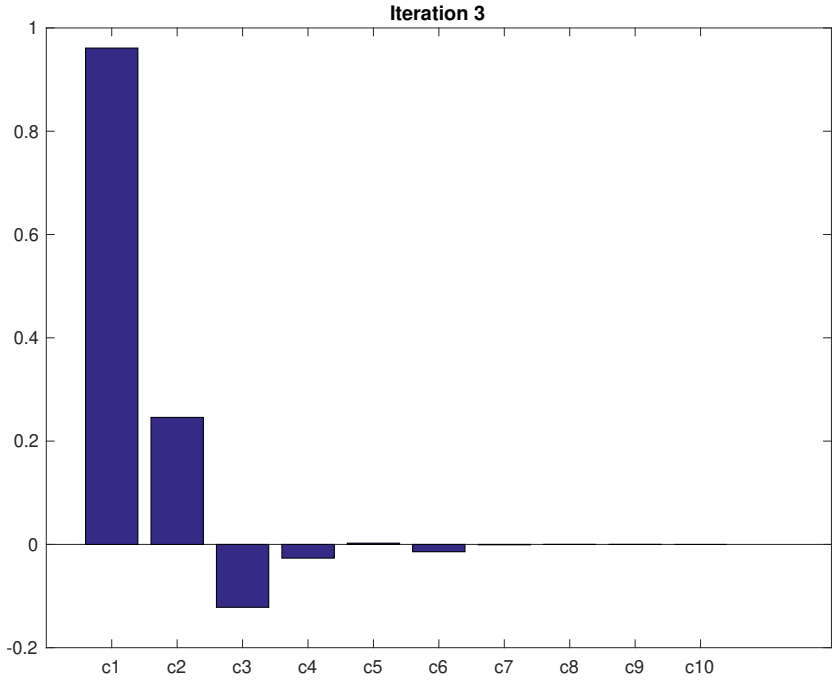

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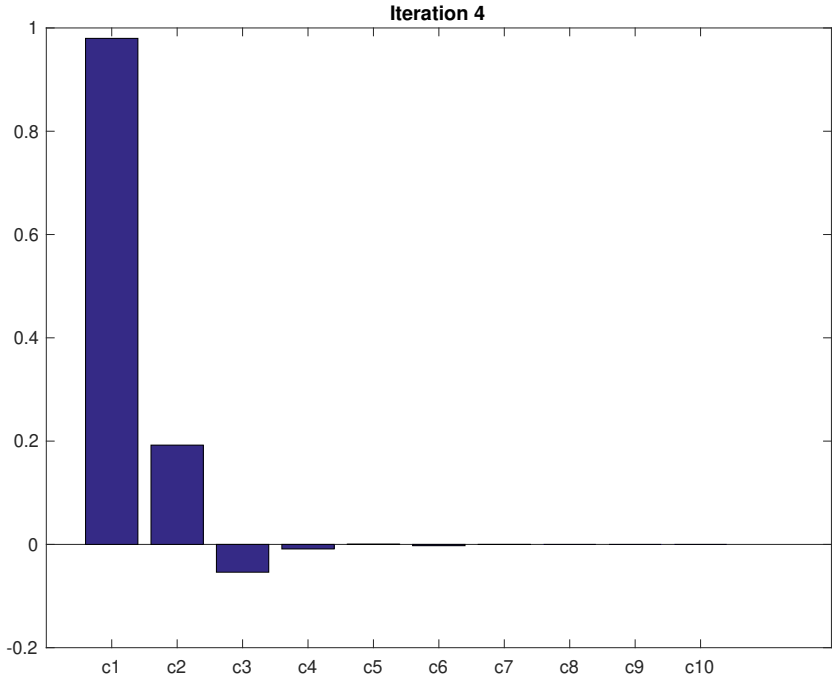

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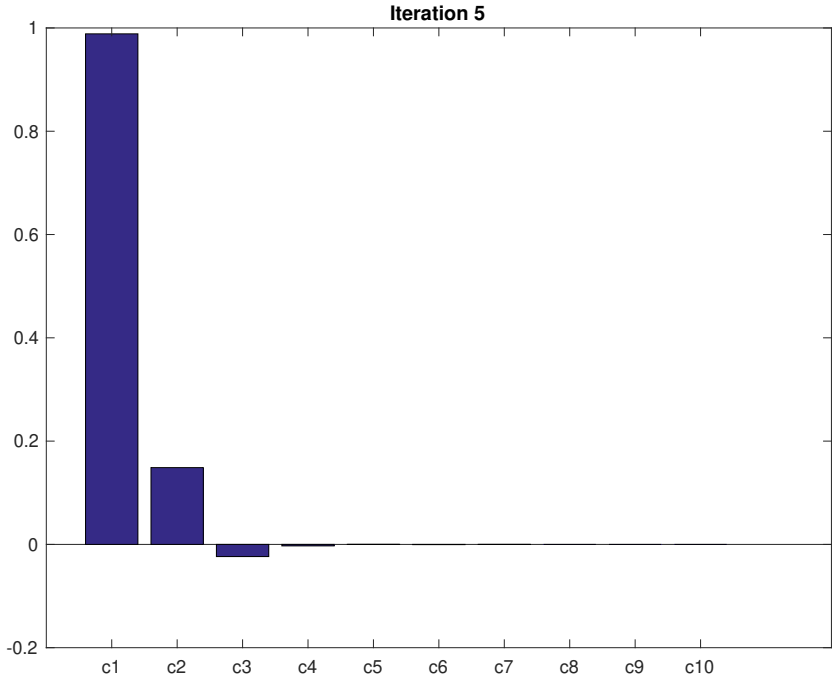

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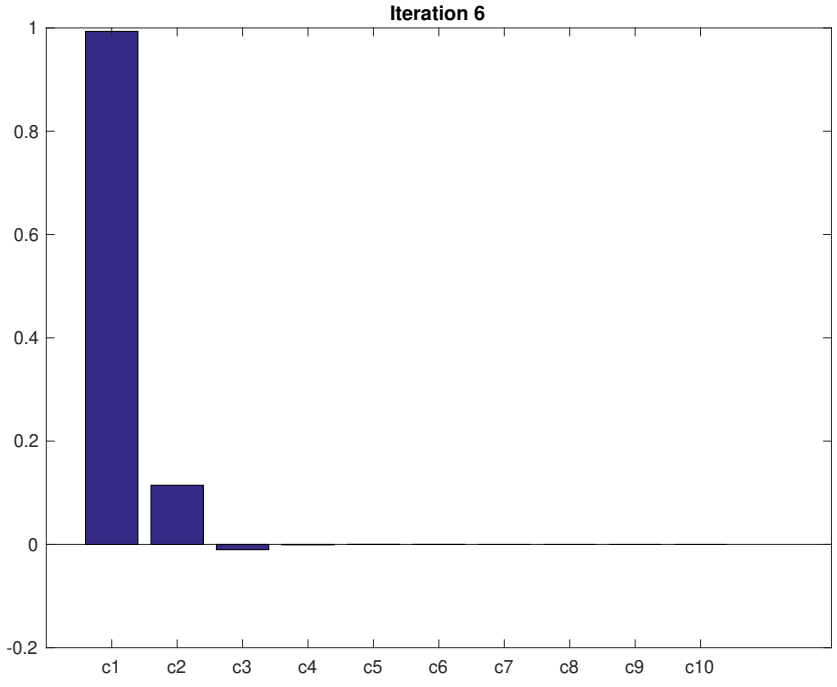

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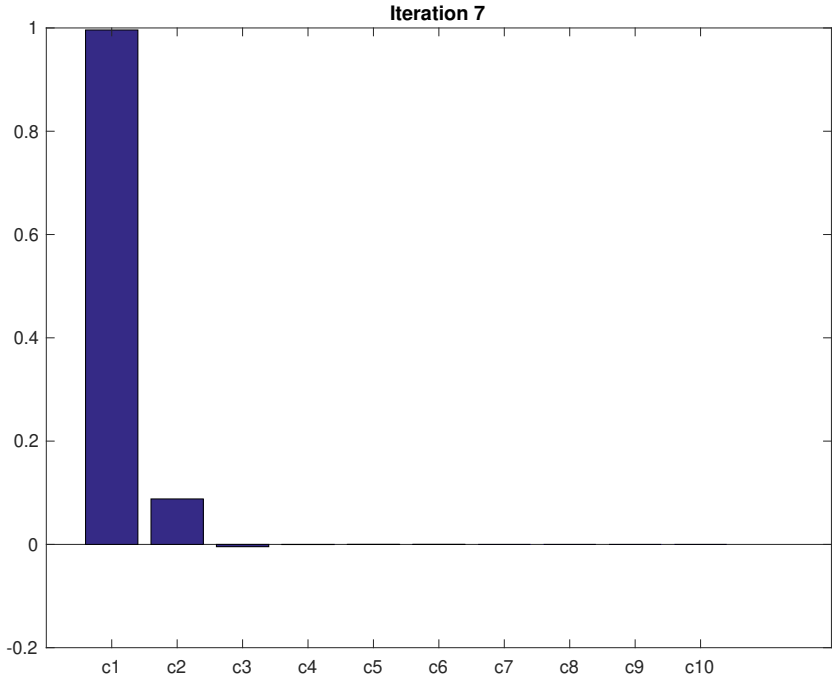

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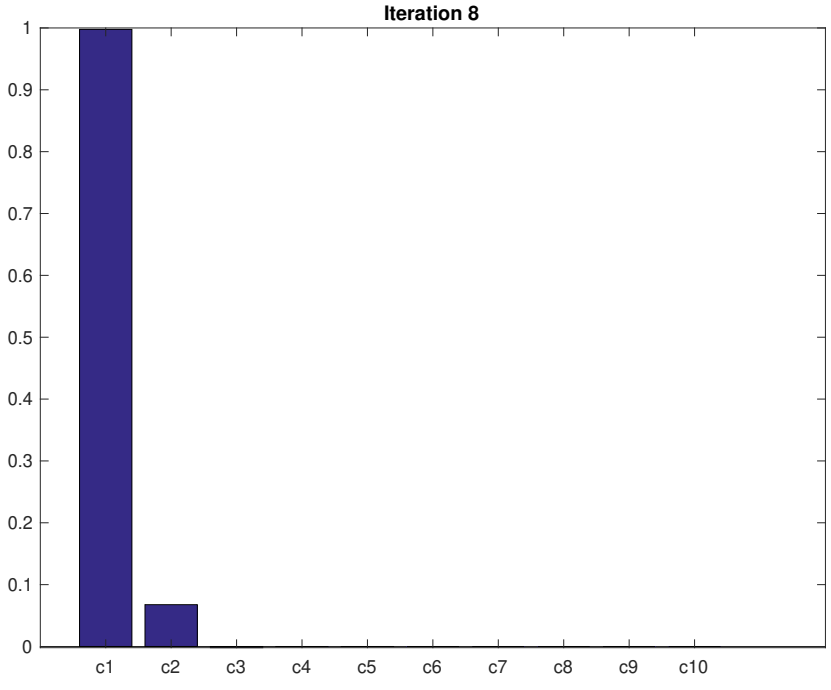

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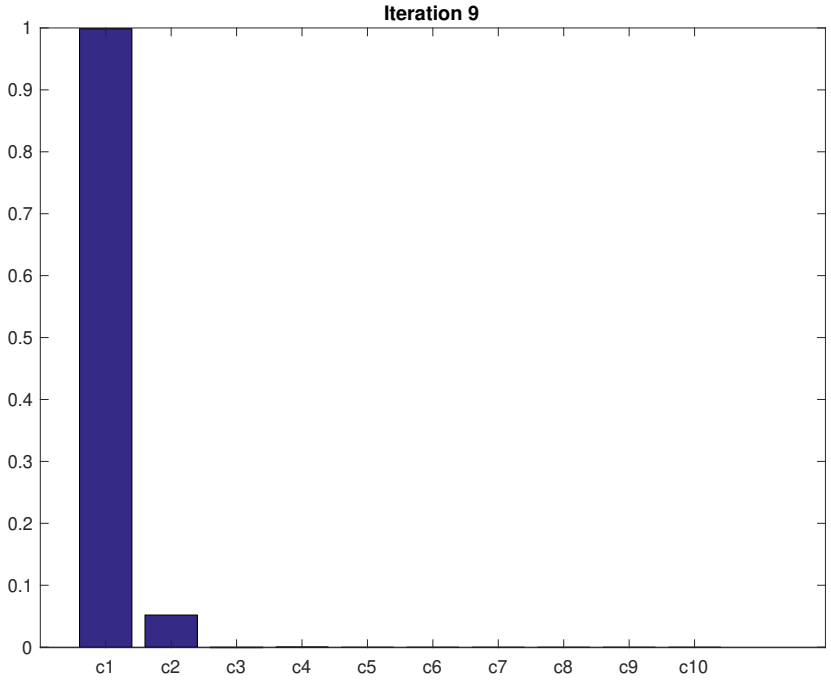

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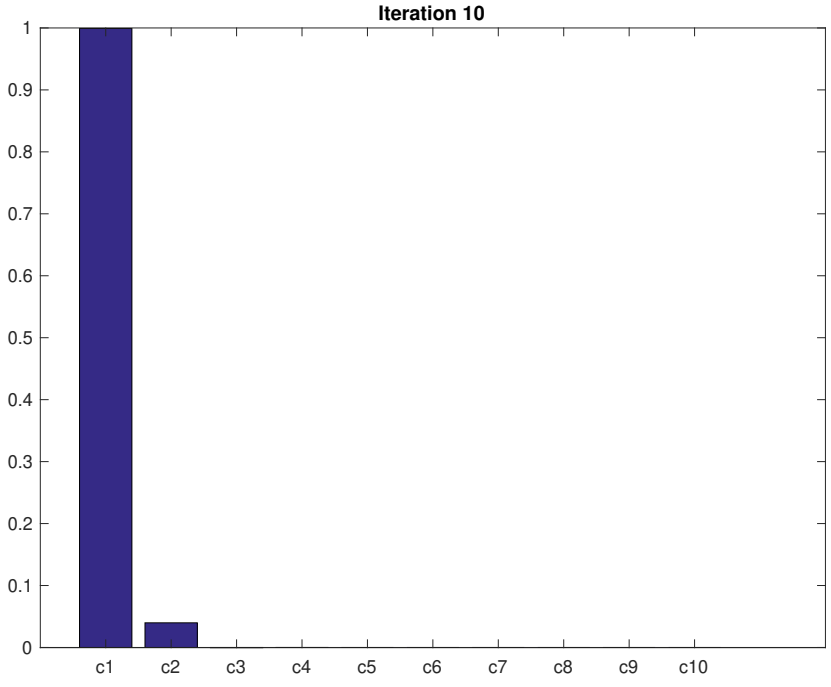

When will convergence be slow? $\lambda_1 \approx \lambda_2$

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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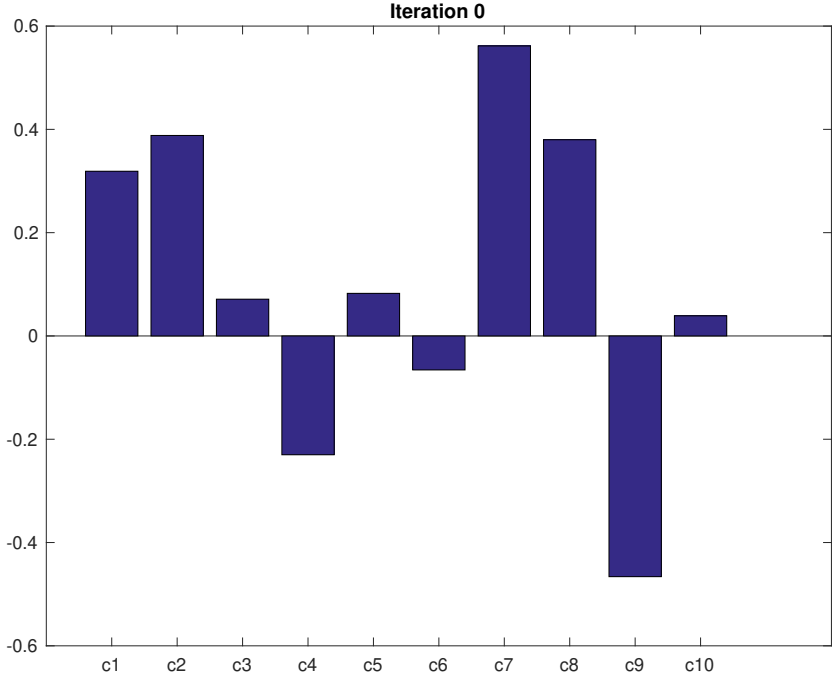

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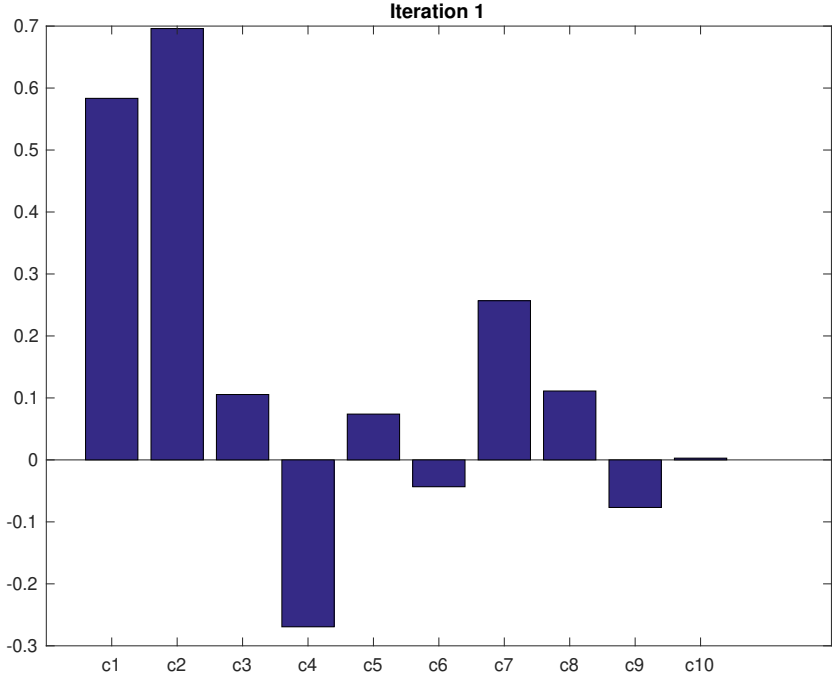

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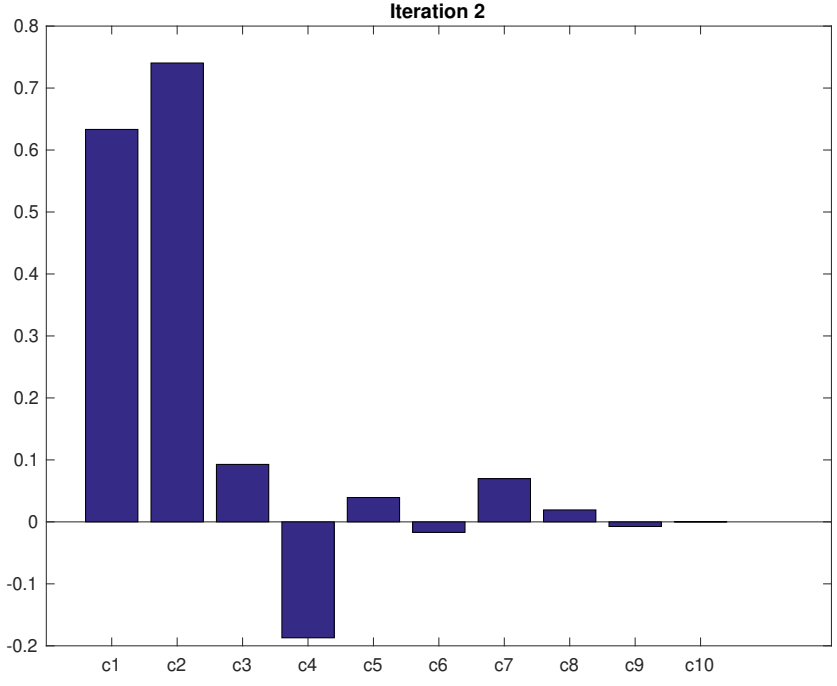

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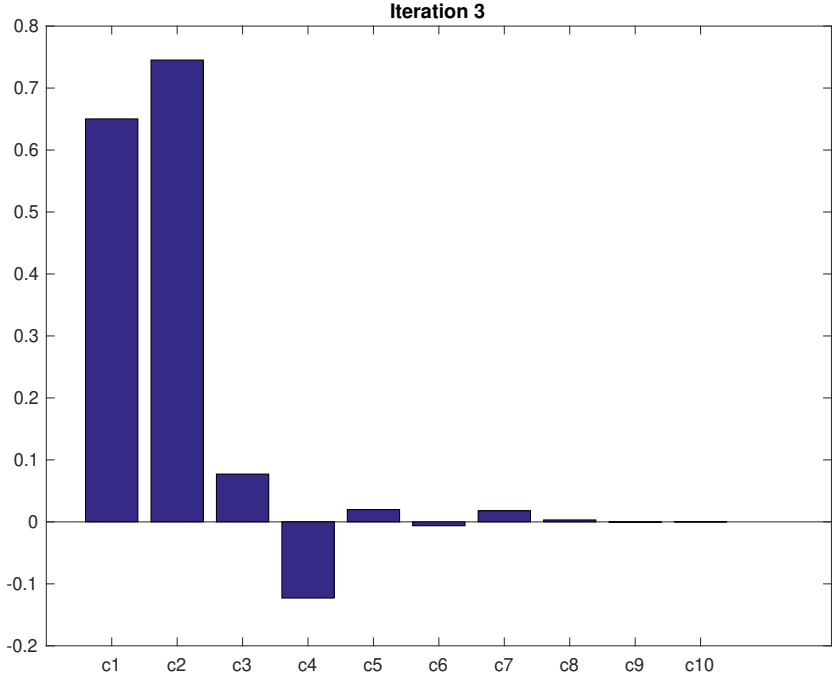

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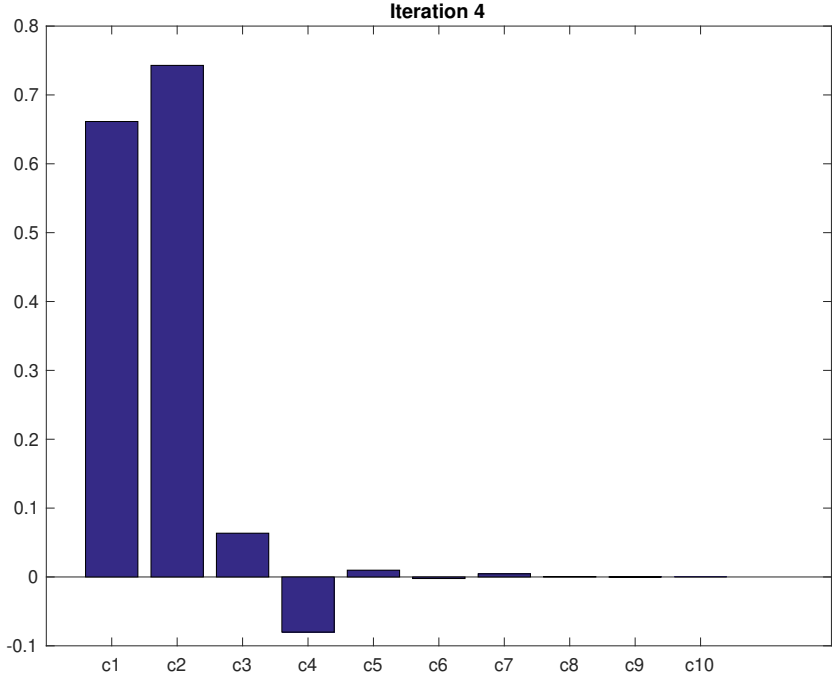

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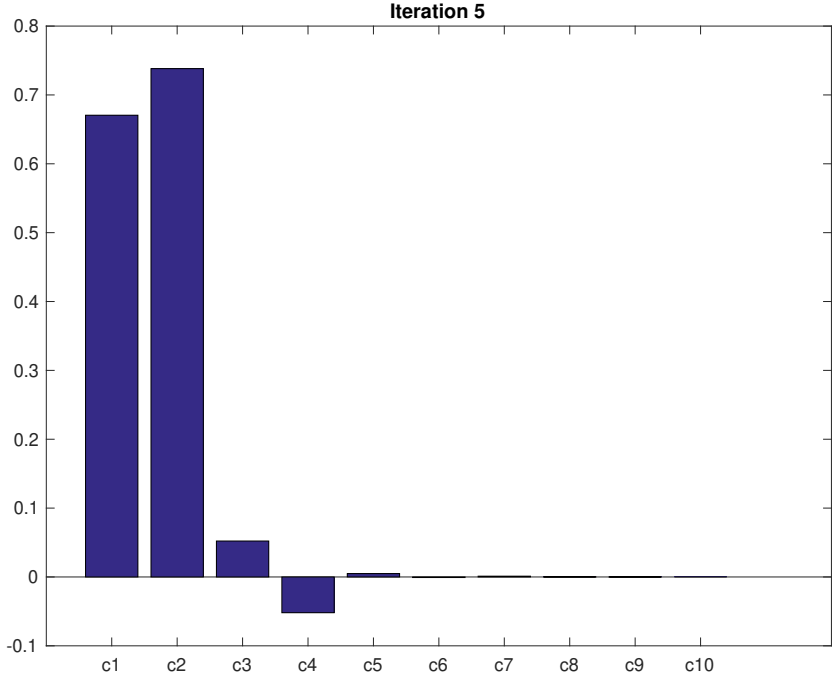

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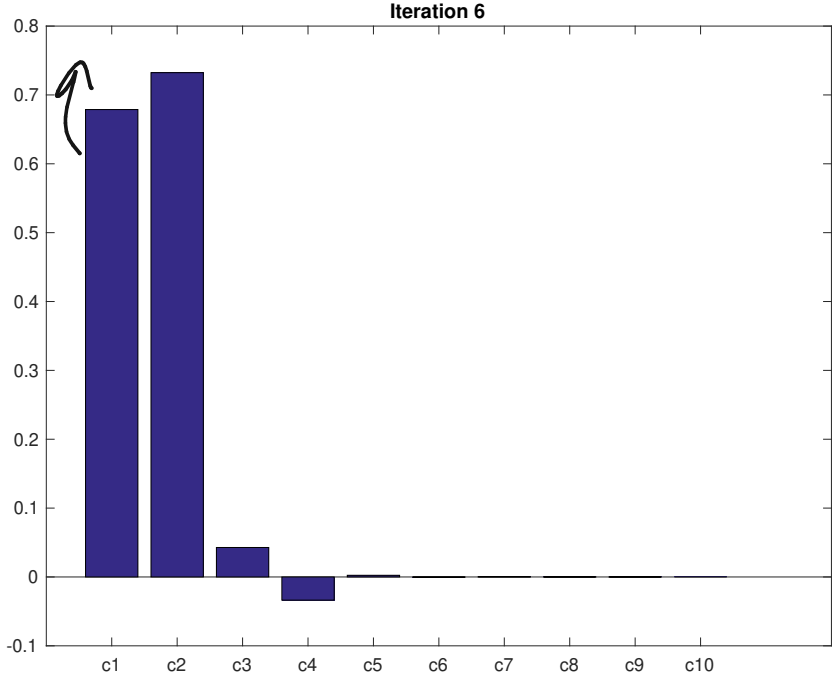

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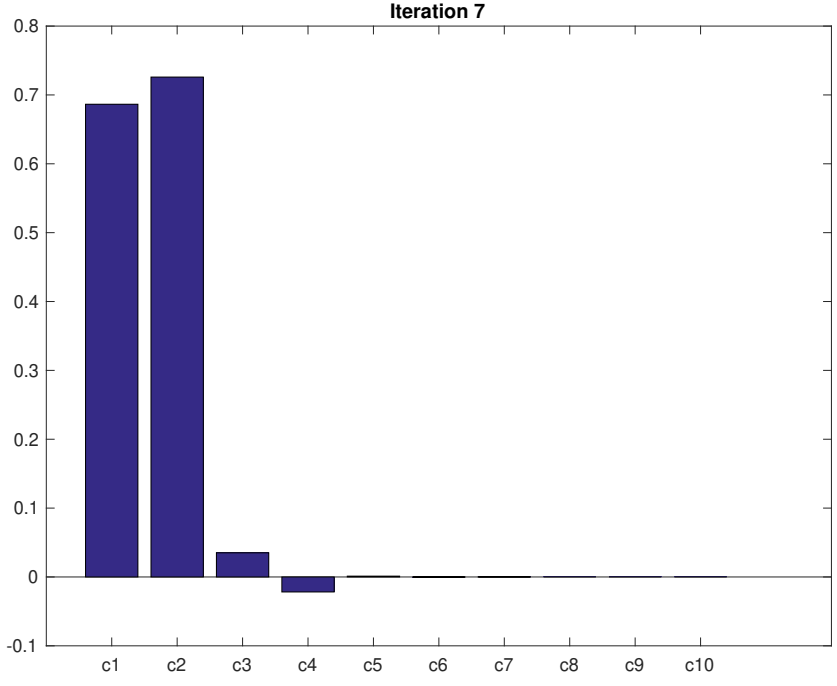

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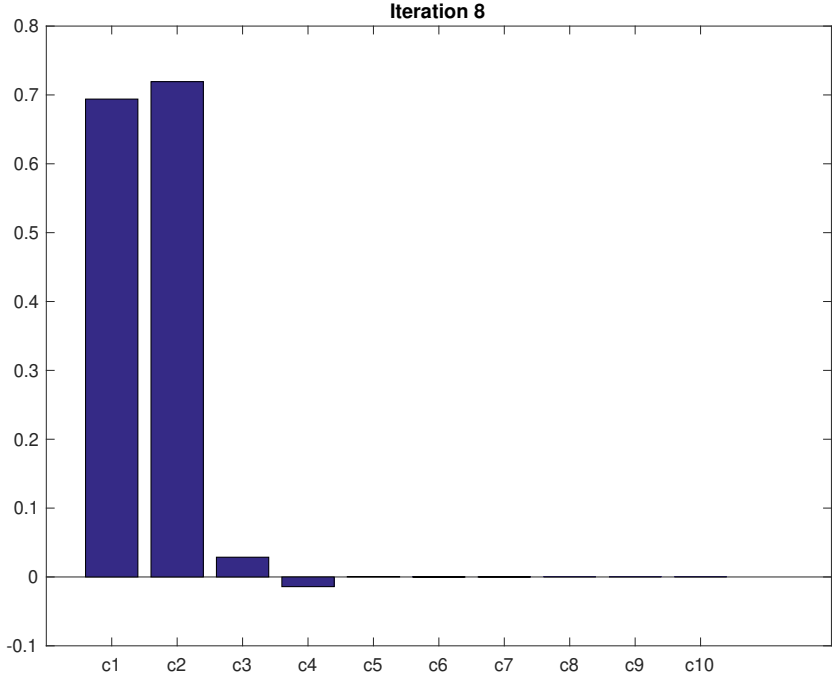

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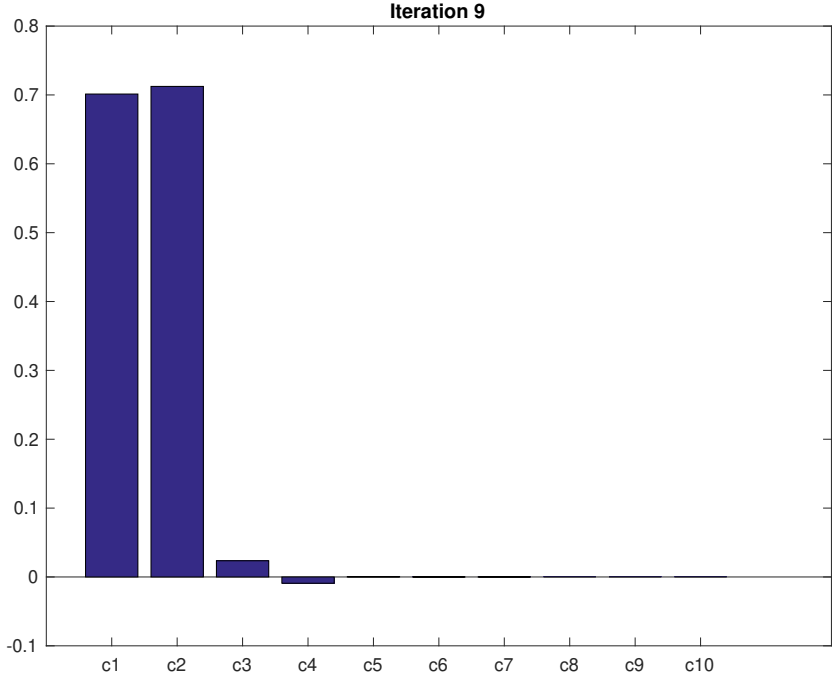

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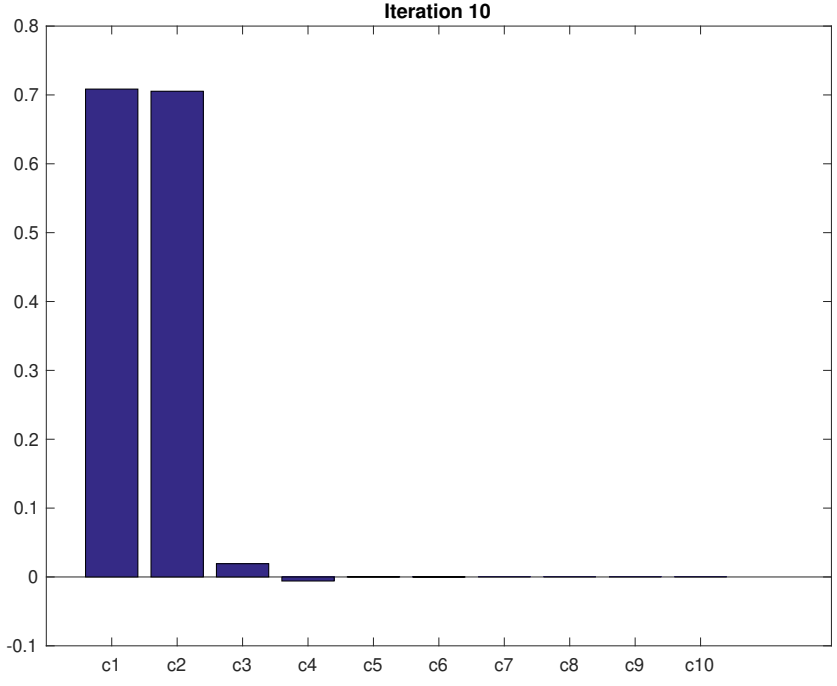

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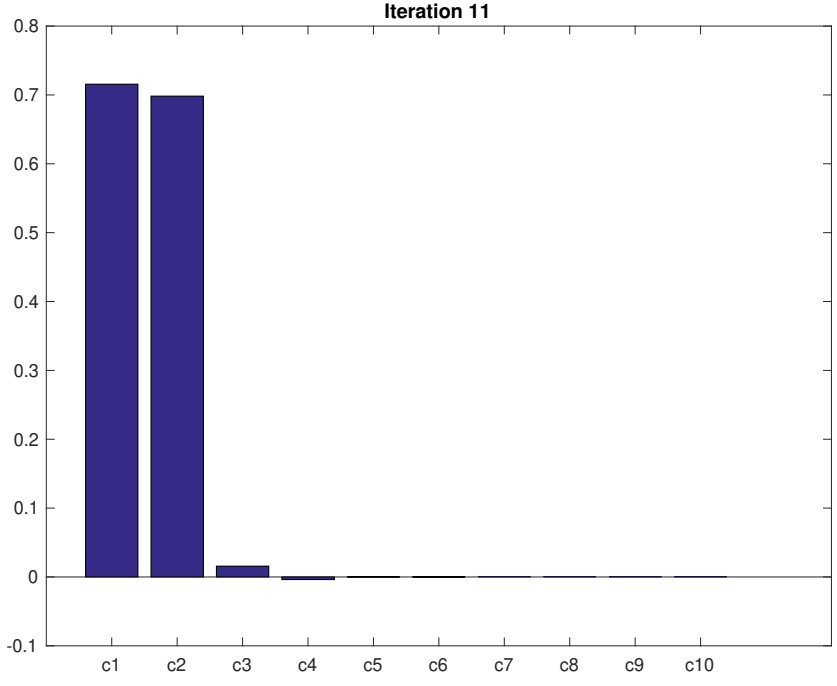

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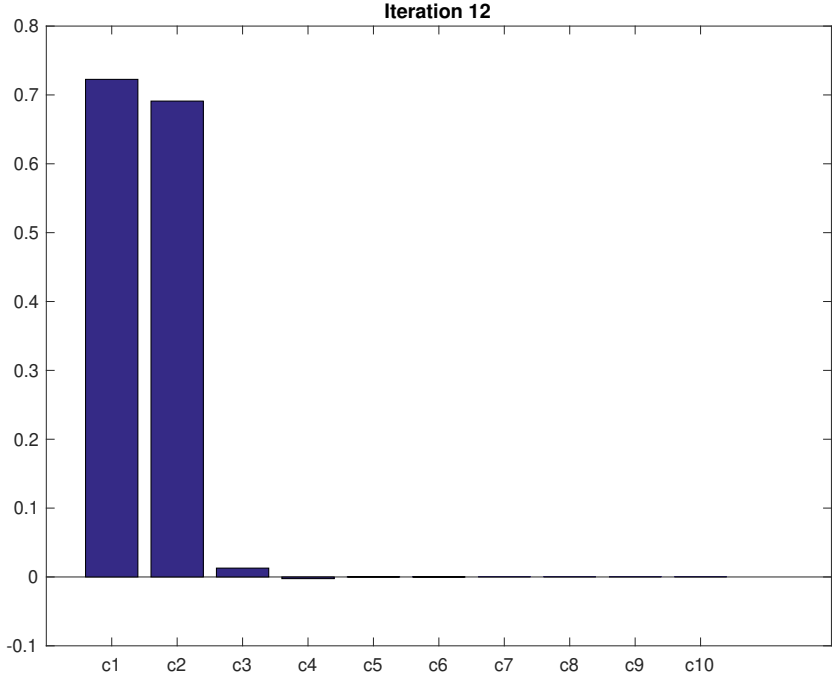

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$\lambda_1 = \lambda_2$

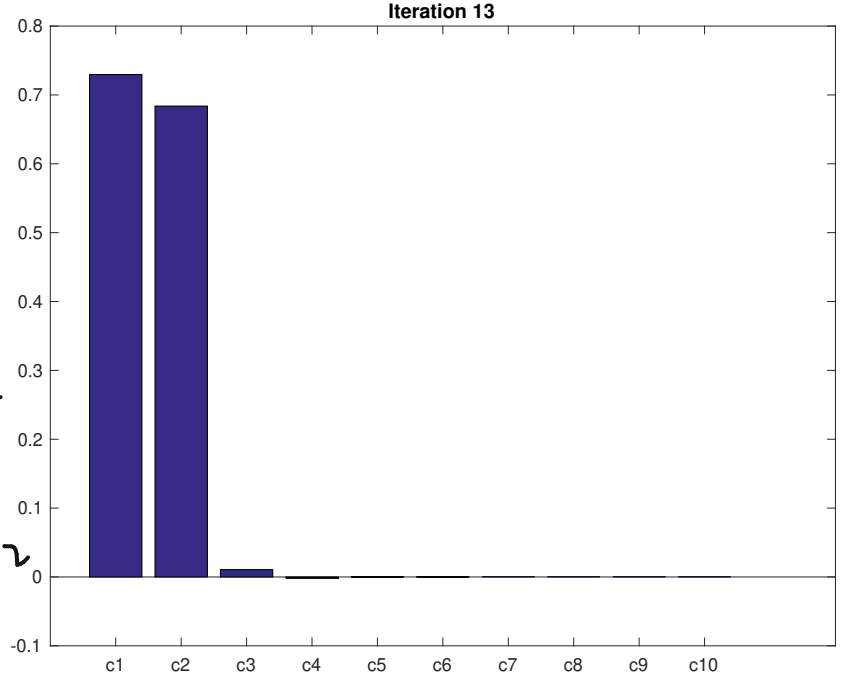
$z = c_1v_1 + c_2v_2$

$Az = Ac_1v_1 + Ac_2v_2$

$= c_1\lambda_1v_1 + c_2\lambda_2v_2$

$= \lambda_1(c_1v_1 + c_2v_2)$

$= \lambda_1 z$



$\lambda_1 > \lambda_2 > \ldots > \lambda_d$

Power Method Convergence Rate

$\lambda_2 = .99\lambda_1 \quad \gamma = .01 \qquad \lambda_2 = \frac{\lambda_1}{3} \quad \gamma = 2/3$

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

Write $|\lambda_2| = (1-\gamma)|\lambda_1|$ for 'gap' $\gamma = \frac{|\lambda_1| - |\lambda_2|}{|\lambda_1|}$. $\quad \gamma \in (0,1)$

How many iterations t does it take to have $|\lambda_2|^t \leq \delta \cdot |\lambda_1|^t$ for $\delta > 0$?

$$\lambda_2^t = \left[(1-\gamma)\lambda_1\right]^t = (1-\gamma)^t \cdot \lambda_1^t \leq \delta \cdot \lambda_1^t$$

$$(1-\gamma)^t \leq \delta$$

$\vec{v}_1$: top eigenvector, being computed, $\vec{z}^{(i)}$: iterate at step i, converging to $\vec{v}_1$. $\lambda_1, \lambda_2, \ldots \lambda_n$: eigenvalues of $\mathbf{A}$, $\gamma = \frac{|\lambda_1| - |\lambda_2|}{|\lambda_1|}$: eigengap controlling convergence rate

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How many iterations t does it take to have $|\lambda_2|^t \leq \delta \cdot |\lambda_1|^t$ for $\delta > 0$?

$$\begin{aligned} |\lambda_2|^t &= (1-\gamma)^t \cdot |\lambda_1|^t \\ &= \underbrace{(1-\gamma)^{1/\gamma \cdot \gamma t}}_{\frac{1}{e}} \cdot |\lambda_1|^t \end{aligned}$$

$\vec{v}_1$: top eigenvector, being computed, $\vec{z}^{(i)}$: iterate at step i, converging to $\vec{v}_1$. $\lambda_1, \lambda_2, \ldots \lambda_n$: eigenvalues of $\mathbf{A}$, $\gamma = \frac{|\lambda_1| - |\lambda_2|}{|\lambda_1|}$: eigengap controlling convergence rate

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$$\begin{aligned} |\lambda_2|^t &= (1-\gamma)^t \cdot |\lambda_1|^t \\ &= (1-\gamma)^{1/\gamma \cdot \gamma t} \cdot |\lambda_1|^t \\ &\leq e^{-\gamma t} \cdot |\lambda_1|^t \end{aligned}$$

$e^{-\gamma t} = \delta$

$-\gamma t = \log(\delta)$

$t = -\frac{\log(\delta)}{\gamma} = \frac{\log(1/\delta)}{\gamma}$

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So it suffices to set $\gamma t = \ln(1/\delta)$. Or $t = \frac{\ln(1/\delta)}{\gamma}$.

$\vec{v}_1$: top eigenvector, being computed, $\vec{z}^{(i)}$: iterate at step i, converging to $\vec{v}_1$. $\lambda_1, \lambda_2, \ldots \lambda_n$: eigenvalues of $\mathbf{A}$, $\gamma = \frac{|\lambda_1| - |\lambda_2|}{|\lambda_1|}$: eigengap controlling convergence rate

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So it suffices to set $\gamma t = \ln(1/\delta)$. Or $t = \frac{\ln(1/\delta)}{\gamma}$.

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 $\vec{v}_1$?

$\vec{v}_1$: top eigenvector, being computed, $\vec{z}^{(i)}$: iterate at step i, converging to $\vec{v}_1$. $\lambda_1, \lambda_2, \ldots \lambda_n$: eigenvalues of $\mathbf{A}$, $\gamma = \frac{|\lambda_1|-|\lambda_2|}{|\lambda_1|}$: eigengap controlling convergence rate

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:

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

$\mathbf{A} \in \mathbb{R}^{d\times d}$: 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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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.

$\mathbf{A} \in \mathbb{R}^{d\times d}$: input with eigenvalues $\lambda_1 \ldots, \lambda_d$ and eigenvectors $\vec{v}_1, \ldots, \vec{v}_d$. $\vec{z}^{(i)}$: iterate at step i. $c_1, \ldots, c_d$: coefficients of $\vec{z}^{(0)}$ in the eigenvector basis.

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$$\vec{z}^{(t)} := \frac{c_1\lambda_1^t\vec{v}_1 + \ldots + c_d\lambda_d^t\vec{v}_d}{\|c_1\lambda_1^t\vec{v}_1 + \ldots + c_d\lambda_d^t\vec{v}_d\|_2}$$

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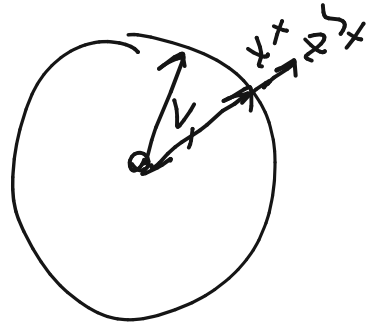
$$\|\vec{z}^{(t)} - \vec{v}_1\|_2 \leq \left\| \frac{c_1\lambda_1^t\vec{v}_1 + \ldots + c_d\lambda_d^t\vec{v}_d}{\|c_1\lambda_1^t\vec{v}_1\|_2} - \vec{v}_1 \right\|_2$$

not quite a unit vector



$A \in \mathbb{R}^{d\times d}$: input with eigenvalues $\lambda_1 \ldots, \lambda_d$ and eigenvectors $\vec{v}_1, \ldots, \vec{v}_d$. $\vec{z}^{(i)}$: iterate at step i. $c_1, \ldots, c_d$: coefficients of $\vec{z}^{(0)}$ in the eigenvector basis.

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

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

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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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Total runtime: $O(t)$ matrix-vector multiplications. If $\mathbf{A} = \mathbf{X}^T\mathbf{X}$:

for $i = 1 \ldots t$
$z^i = A z^{i-1}$

$$O\left(\text{mv}(\mathbf{X}) \cdot \frac{\ln(d/\epsilon)}{\gamma} \cdot\right) = O\left(nd \cdot \frac{\ln(d/\epsilon)}{\gamma}\right).$$

$O(nd^2)$

$(X^T(X z^{i-1}))$

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How is ϵ dependence?

How is γ dependence?

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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$p(x) = x^t$

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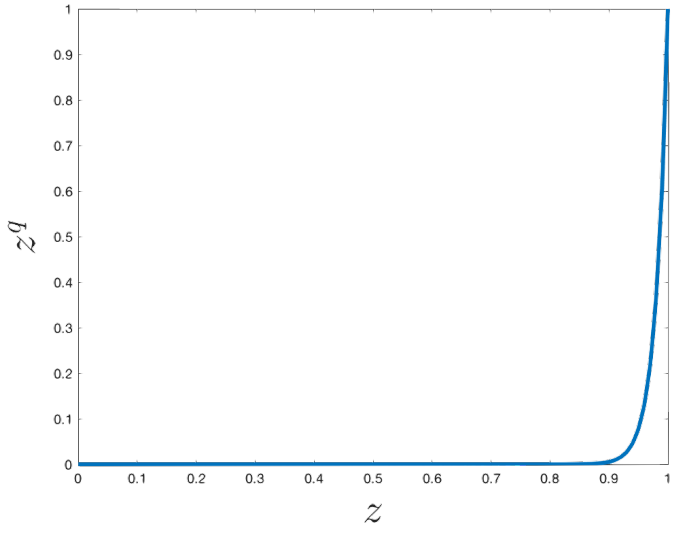
- Krylov methods: apply a better degree t polynomial $T_t(\cdot)$ to the eigenvalues to separate $T_t(\lambda_1)$ from $T_t(\lambda_i)$.
- Still requires just t matrix vector multiplies. Why?

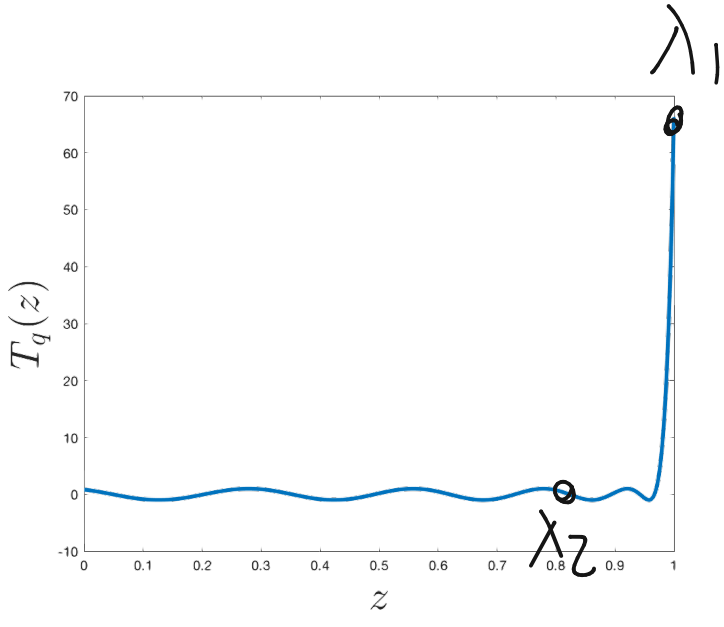
$$\left(A\left(A\left(A z^0\right)\right)\right)$$

$$c_t A^t z^0 + \ldots + c_2 A^2 z^0 + c_1 A z^0 + c_0 z^0 = p(A) \cdot z^0$$

krylov subspace methods



vs.



Optimal 'jump' polynomial in general is given by a degree t Chebyshev polynomial. Krylov methods find a polynomial tuned to the input matrix that does at least as well.

Generalizations to Larger k

- Block Power Method (a.k.a. Simultaneous Iteration, Subspace Iteration, or Orthogonal Iteration)
- Pick random block of vectors $\mathbf{Z}^{(0)} \in \mathbb{R}^{n \times k}$. $\mathbf{Z}^{(i)} = \mathbf{orth}(\mathbf{A}\mathbf{Z}^{(i-1)})$.
- Block Krylov methods use an analogous approach.

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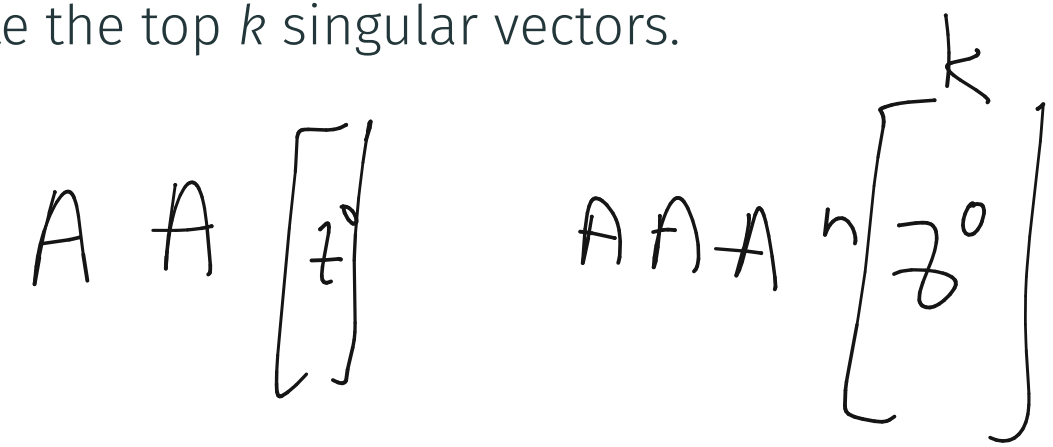
to accurately compute the top k singular vectors.



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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.