Orthogonal tensor decomposition

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Largely based on 2012 arXiv report “Tensor decompositions for learning latent variable models”, with Anandkumar, Ge, Kakade, and Telgarsky.

1. The basic decomposition problem

The basic decomposition problem

Notation: For a vector $\vec{x} = (x_1, x_2, \ldots, x_n) \in \mathbb{R}^n$,

$$\vec{x} \otimes \vec{x} \otimes \vec{x}$$

denotes the 3-way array (call it a "tensor") in $\mathbb{R}^{n \times n \times n}$ whose $(i, j, k)^{\text{th}}$ entry is $x_i x_j x_k$.

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Problem: Given $T \in \mathbb{R}^{n \times n \times n}$ with the promise that

$$T = \sum_{t=1}^{n} \lambda_t \, \vec{v}_t \otimes \vec{v}_t \otimes \vec{v}_t$$

for some orthonormal basis $\{\vec{v}_t\}$ of $\mathbb{R}^n$ (w.r.t. standard inner product) and positive scalars $\{\lambda_t > 0\}$, approximately find $\{(\vec{v}_t, \lambda_t)\}$ (up to some desired precision).

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2. If so, is there an efficient algorithm for finding the decomposition?
3. What if T is perturbed by some small amount?

> Perturbed problem: Same as the original problem, except instead of T, we are given $T + E$ for some "error tensor" E.

How "large" can E be if we want ε precision?

Analogous matrix problem

Matrix problem: Given $M \in \mathbb{R}^{n \times n}$ with the promise that

$$M = \sum_{t=1}^{n} \lambda_t \, \vec{v}_t \, \vec{v}_t^{\top}$$

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  Answer provided by **matrix perturbation theory** (*e.g.*, Davis-Kahan), which requires $\|E\|_2 < \min_{i \neq j} |\lambda_i - \lambda_j|$.

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Where the decompositions do exist, the Perturbed problem asks if they are "robust".

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- Why?: $T - \lambda_t \, \vec{v}_t \otimes \vec{v}_t \otimes \vec{v}_t \; = \; \sum_{\tau \neq t} \lambda_\tau \, \vec{v}_\tau \otimes \vec{v}_\tau \otimes \vec{v}_\tau$.

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- Catch: We don't recover $(\vec{v}_t, \lambda_t)$ exactly, so we actually can only replace T with

$$T - \lambda_t\ \vec{v}_t \otimes \vec{v}_t \otimes \vec{v}_t + E_t$$

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  for some "error tensor" E_t.
- Therefore, must anyway deal with perturbations.

Rest of this talk

1. Identifiability of decomposition $\{(\vec{v}_t, \lambda_t)\}$ from T.
2. A decomposition algorithm based on tensor power iteration.
3. Error analysis of decomposition algorithm.

2. Identifiability

Identifiability of the decomposition

Orthonormal basis $\{\vec{v}_t\}$ of $\mathbb{R}^n$, positive scalars $\{\lambda_t > 0\}$:

$$T = \sum_{t=1}^{n} \lambda_t \, \vec{v}_t \otimes \vec{v}_t \otimes \vec{v}_t$$

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In what sense is $\{(\vec{v}_t, \lambda_t)\}$ uniquely determined?

Claim: $\{\vec{v}_t\}$ are isolated local maximizers of certain cubic form $f_T : \mathbb{S}^{n-1} \to \mathbb{R}^n$, and $f_T(\vec{v}_t) = \lambda_t$.

Aside: multilinear form

There is a natural trilinear form associated with T:

$$(\vec{x}, \vec{y}, \vec{z}) \mapsto \sum_{i,j,k} T_{i,j,k}\, x_i y_j z_k .$$

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$$(\vec{x}, \vec{y}) \mapsto \sum_{i,j} M_{i,j}\, x_i y_j = \vec{x}^\top M \vec{y}.$$

Review: Rayleigh quotient

Recall Rayleigh quotient for matrix $M := \sum_{t=1}^{n} \lambda_t \, \vec{v}_t \vec{v}_t^{\top}$ (assuming $\vec{x} \in \mathbb{S}^{n-1}$):

$$R_M(\vec{x}) \;:=\; \vec{x}^{\top} M \vec{x} \;=\; \sum_{t=1}^{n} \lambda_t \, (\vec{v}_t^{\top} \vec{x})^2 .$$

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Every $\vec{v}_t$ such that $|\lambda_t| = \max!$ is a maximizer of R_M.

(These are also the only local maximizers.)

The natural cubic form

Consider the function $f_T : \mathbb{S}^{n-1} \to \mathbb{R}^n$ given by

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$$f_T(\vec{x}) = \sum_{t=1}^{n} \lambda_t \sum_{i,j,k} \left(\vec{v}_t \otimes \vec{v}_t \otimes \vec{v}_t\right)_{i,j,k} x_i x_j x_k$$

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Observation: $f_T(\vec{v}_t) = \lambda_t$.

Variational characterization

Claim: Isolated local maximizers of f_T on $\mathbb{S}^{n-1}$ are $\{\vec{v}_t\}$.

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Second-order condition for isolated local maxima:

$$\vec{w}^{\top} \left(2 \sum_{t=1}^{n} \lambda_t \, (\vec{v}_t^{\top} \vec{x}) \vec{v}_t \vec{v}_t^{\top} - \lambda I \right) \vec{w} < 0, \qquad \vec{w} \perp \vec{x}.$$

Intuition behind variational characterization

May as well assume $\vec{v}_t$ is t^{th} coordinate basis vector, so

$$\max_{\vec{x} \in \mathbb{R}^n} f_T(\vec{x}) = \sum_{t=1}^{n} \lambda_t \, x_t^3 \quad \text{s.t.} \quad \sum_{t=1}^{n} x_t^2 = 1.$$

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$$f_T(\vec{x}) = \lambda_1 x_1^3 + \lambda_2 x_2^3 < \lambda_1 x_1^2 + \lambda_2 x_2^2 \leq \max\{\lambda_1, \ \lambda_2\}.$$

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Better to have $|\text{supp}(\vec{x})| = 1$, *i.e.*, picking $\vec{x}$ to be a coordinate basis vector. ∎

Aside: canonical polyadic decomposition

Rank-K **canonical polyadic decomposition** (CPD) of T
(also called PARAFAC, CANDECOMP, or CP):

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N.B.: *Overcomplete* ($K > n$) CPD is also interesting *and a possibility* as long as $K(3n + 1) \ll n^3$.

3. Power iteration

The quadratic operator

Easy claim: Repeated application of a certain quadratic operator (based on T) recovers a single $(\lambda_t, \vec{v}_t)$ up to any desired precision.

For any $A \in \mathbb{R}^{n\times n\times n}$ and $\vec{x} = (x_1, x_2, \ldots, x_n) \in \mathbb{R}^n$, define the quadratic operator

$$\phi_A(\vec{x}) := \sum_{i,j,k} A_{i,j,k}\, x_j x_k\, \vec{e}_i \ \in \mathbb{R}^n$$

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$$\text{If } T = \sum_{t=1}^{n} \lambda_t \, \vec{v}_t \otimes \vec{v}_t \otimes \vec{v}_t \,, \ \text{ then } \phi_T(\vec{x}) = \sum_{t=1}^{n} \lambda_t \, \left(\vec{v}_t^{\top} \vec{x}\right)^2 \vec{v}_t .$$

An algorithm?

Recall: First-order condition for local maxima of $f_T(\vec{x}) = \sum_{t=1}^{n} \lambda_t \, (\vec{v}_t^\top \vec{x})^3$ for $\vec{x} \in \mathbb{S}^{n-1}$:

$$\phi_T(\vec{x}) = \sum_{t=1}^{n} \lambda_t \, (\vec{v}_t^\top \vec{x})^2 \, \vec{v}_t = \lambda \vec{x}$$

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N.B.: Gradient ascent also works [Kolda & Mayo, ’11].

Tensor power iteration

Start with some $\vec{x}^{(0)}$, and for $j = 1, 2, \ldots$:

$$\vec{x}^{(j)} \ := \ \phi_T\left(\vec{x}^{(j-1)}\right) \ = \ \sum_{t=1}^{n} \lambda_t \left(\vec{v}_t^{\top} \vec{x}^{(j-1)}\right)^2 \vec{v}_t .$$

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Claim: For almost all initial $\vec{x}^{(0)}$, the sequence $\big(\vec{x}^{(j)} / \|\vec{x}^{(j)}\|\big)_{j=1}^{\infty}$ converges *quadratically fast* to some $\vec{v}_t$.

Review: matrix power iteration

Recall matrix power iteration for matrix $M := \sum_{t=1}^{n} \lambda_t \, \vec{v}_t \vec{v}_t^{\top}$:

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$$\vec{x}^{(i)} := M\vec{x}^{(j-1)} = \sum_{t=1}^{n} \lambda_t \left(\vec{v}_t^{\top} \vec{x}^{(j-1)} \right) \vec{v}_t .$$

i.e., component in $\vec{v}_t$ direction is scaled by λ_t.

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i.e., component in $\vec{v}_t$ direction is scaled by λ_t.

If $\lambda_1 > \lambda_2 \geq \cdots$, then

$$\frac{\left(\vec{v}_1^{\top} \vec{x}^{(j)}\right)^2}{\sum_{t=1}^{n} \left(\vec{v}_t^{\top} \vec{x}^{(j)}\right)^2} \geq 1 - k\left(\frac{\lambda_2}{\lambda_1}\right)^{2j} .$$

i.e., converges *linearly* to $\vec{v}_1$ (assuming gap $\lambda_2/\lambda_1 < 1$).

Tensor power iteration convergence analysis

Let $c_t := \vec{v}_t^\top \vec{x}^{(0)}$ (initial component in $\vec{v}_t$ direction); assume WLOG

$$\lambda_1 |c_1| > \lambda_2 |c_2| \geq \lambda_3 |c_3| \geq \cdots .$$

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Then

$$\vec{x}^{(1)} = \sum_{t=1}^{n} \lambda_t \left(\vec{v}_t^{\top} \vec{x}^{(0)} \right)^2 \vec{v}_t = \sum_{t=1}^{n} \lambda_t c_t^2 \, \vec{v}_t$$

i.e., component in $\vec{v}_t$ direction is squared then scaled by λ_t.

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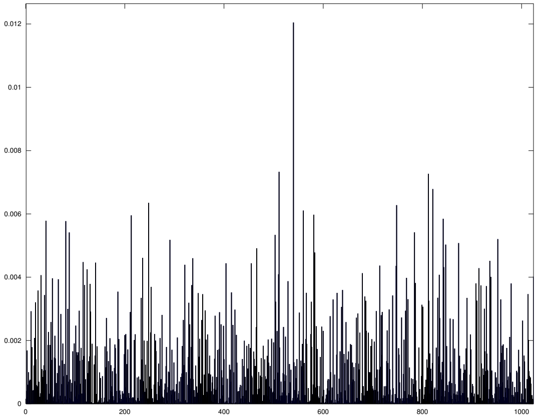
Easy to show

$$\frac{\left(\vec{v}_1{}^\top \vec{x}^{(j)} \right)^2}{\sum_{t=1}^{n} \left(\vec{v}_t{}^\top \vec{x}^{(j)} \right)^2} \geq 1 - k \left(\frac{\lambda_1}{\max_{t \neq 1} \lambda_t} \right)^2 \left| \frac{\lambda_2 c_2}{\lambda_1 c_1} \right|^{2^{j+1}} .$$

Example

$$n = 1024,\ \lambda_t \sim_{\text{u.a.r.}} [0, 1].$$



Value of $(\vec{v}_t^{\top} \vec{x}^{(0)})^2$ for $t = 1, 2, \ldots, 1024$

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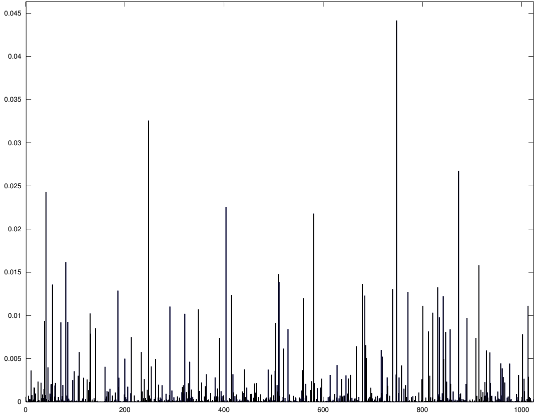

Value of $(\vec{v}_t^{\top} \vec{x}^{(1)})^2$ for $t = 1, 2, \ldots, 1024$

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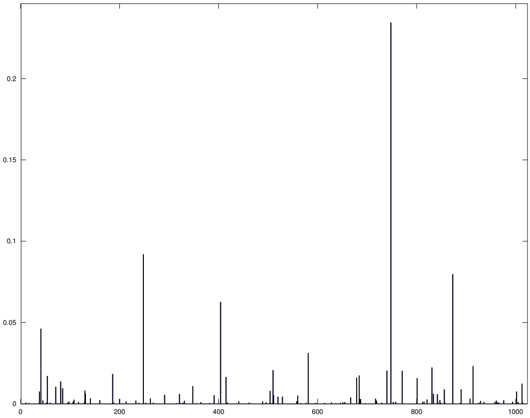

Value of $(\vec{v}_t^\top \vec{x}^{(2)})^2$ for $t = 1, 2, \ldots, 1024$

Example

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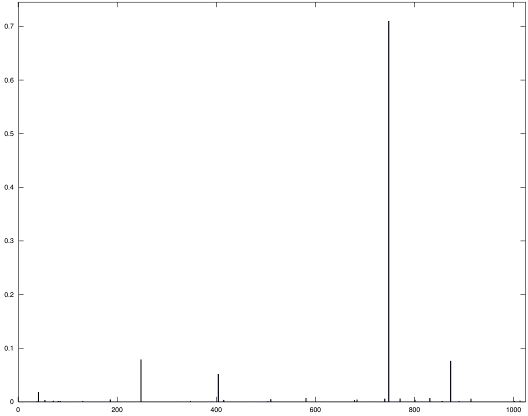

Value of $(\vec{v}_t^\top \vec{x}^{(3)})^2$ for $t = 1, 2, \ldots, 1024$

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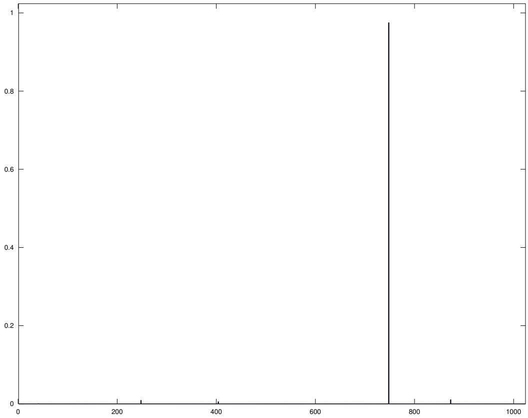

Value of $(\vec{v}_t^{\top} \vec{x}^{(4)})^2$ for $t = 1, 2, \ldots, 1024$

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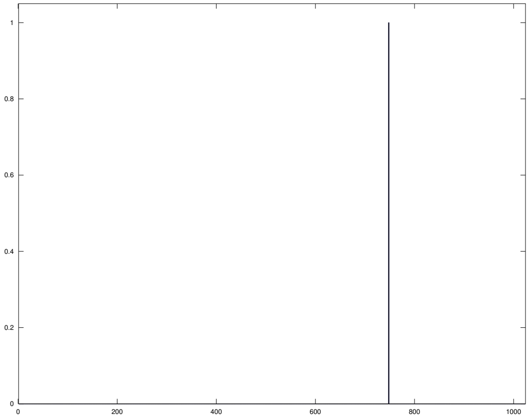

Value of $(\vec{v}_t^{\top} \vec{x}^{(5)})^2$ for $t = 1, 2, \ldots, 1024$

Matrix vs. tensor power iteration

Matrix power iteration:

Tensor power iteration:

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1. Requires gap between largest and second-largest λ_t.
   (Property of the matrix only.)

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Matrix power iteration:

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3. Linear convergence. (Need $O(\log(1/\epsilon))$ iterations.)

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3. Quadratic convergence. (Need $O(\log\log(1/\epsilon))$ iterations.)

Initialization of tensor power iteration

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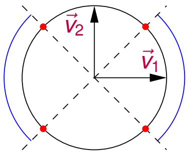
Fortunately, bad initialization points are atypical.



Full decomposition algorithm

Input: $T \in \mathbb{R}^{n \times n \times n}$.

Initialize: $\widetilde{T} := T$.

For $i = 1, 2, \ldots, n$:

1. Pick $\vec{x}^{(0)} \in \mathbb{S}^{n-1}$ u.a.r.
2. Run tensor power iteration with $\widetilde{T}$ starting from $\vec{x}^{(0)}$ for N iterations.
3. Set $\hat{v}_i := \vec{x}^{(N)} / \|\vec{x}^{(N)}\|$ and $\hat{\lambda}_i := f_{\widetilde{T}}(\hat{v}_i)$.
4. Replace $\widetilde{T} := \widetilde{T} - \hat{\lambda}_i \, \hat{v}_i \otimes \hat{v}_i \otimes \hat{v}_i$.

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Actually: repeat Steps 1–3 several times, and take results of trial yielding largest $\hat{\lambda}_i$.

Aside: direct minimization

Can also consider directly minimizing

$$\left\| T - \sum_{t=1}^{n} \hat{\lambda}_t \; \hat{v}_t \otimes \hat{v}_t \otimes \hat{v}_t \right\|_F^2$$

via local optimization (*e.g.*, block coordinate descent).

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Decomposition algorithm via tensor power iteration can be viewed as **orthgonal greedy algorithm** for minimizing above objective [Zhang & Golub, '01].

Aside: implementation for bag-of-words models

Let $\vec{f}^{(i)}$ be empirical word frequency vector for document i:

$$\vec{f}_j^{(i)} = \frac{\text{\# times word } j \text{ appears in document } i}{\text{length of document } i}$$

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$$\widehat{\text{Pairs}} \approx \frac{1}{m} \sum_{i=1}^{m} \vec{f}^{(i)} \otimes \vec{f}^{(i)} \longrightarrow \sum_{t=1}^{K} \vec{\mu}_t \otimes \vec{\mu}_t .$$

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Use inner product system given by $\langle \vec{x}, \vec{y} \rangle := \vec{x}^\top \widehat{\text{Pairs}}^\dagger \vec{y}$.

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Final running time $\propto$ # topics $\times$ (model size $+$ input size).

4. Error analysis

Effect of errors in tensor power iterations

Suppose we are given $\widehat{T} := T + E$, with

$$T = \sum_{t=1}^{n} \lambda_t \, \vec{v}_t \otimes \vec{v}_t \otimes \vec{v}_t, \qquad \varepsilon := \sup_{\vec{x} \in \mathbb{S}^{n-1}} \|\phi_E(\vec{x})\|.$$

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What can we say about the resulting $\hat{v}_i$ and $\hat{\lambda}_i$?

Perturbation analysis

Theorem: If $\varepsilon \leq O(\frac{\min_t \lambda_t}{n})$, then with high probability, a modified variant of the full decomposition algorithm returns $\{(\hat{v}_i, \hat{\lambda}_i) : i \in [n]\}$ with

$$\|\hat{v}_i - \vec{v}_i\| \leq O(\varepsilon/\lambda_i), \qquad |\hat{\lambda}_i - \lambda_i| \leq O(\varepsilon), \qquad i \in [n].$$

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Essentially third-order analogue of Wedin's theorem for SVD of matrices, but specific to particular algorithm.

Effect of errors in tensor power iterations

Quadratic operator $\phi_{\widehat{T}}$ with $\widehat{T}$:

$$\phi_{\widehat{T}}(\vec{x}) \;=\; \sum_{t=1}^{n} \lambda_t \left(\vec{v}_t^{\top}\vec{x}\right)^2 \vec{v}_t \;+\; \phi_E(\vec{x}).$$

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Claim: If $\varepsilon \leq O(\frac{\min_t \lambda_t}{n})$ and $N \geq \Omega(\log(n) + \log\log \frac{\max_t \lambda_t}{\varepsilon})$, then N steps of tensor power iteration on $T + E$ (with good initialization) gives

$$\|\hat{v}_i - \vec{v}_i\| \leq O(\varepsilon/\lambda_i), \qquad |\hat{\lambda}_i - \lambda_i| \leq O(\varepsilon).$$

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(For simplicity, assume $\lambda_1 = \cdots = \lambda_n = 1$.)

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Approximate (say) $\vec{v}_1$ with $\hat{v}_1$ up to error $\|\vec{v}_1 - \hat{v}_1\| \leq \varepsilon$.

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Deflation danger: To find next $\vec{v}_t$, use

$$\widehat{T} - \hat{v}_1 \otimes \hat{v}_1 \otimes \hat{v}_1 = \sum_{t=2}^{n} \vec{v}_t \otimes \vec{v}_t \otimes \vec{v}_t + E + \left(\vec{v}_1 \otimes \vec{v}_1 \otimes \vec{v}_1 - \hat{v}_1 \otimes \hat{v}_1 \otimes \hat{v}_1\right).$$

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Now error seems to be of size 2ε . . .

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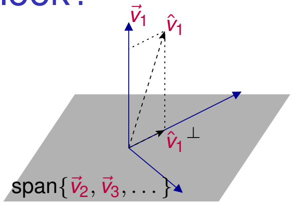
Now error seems to be of size $2\varepsilon \ldots$ exponential explosion?

How do the errors look?



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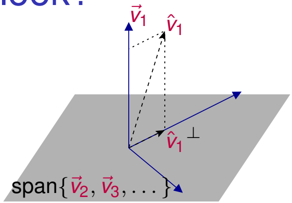

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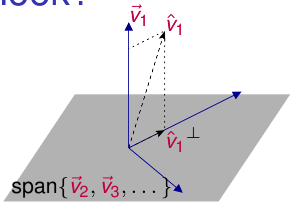

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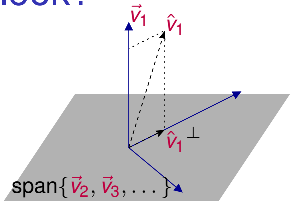

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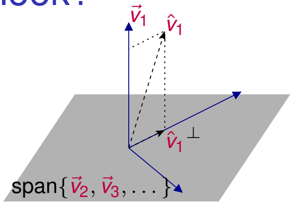

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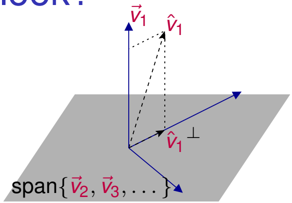

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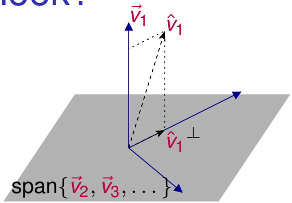

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- Effect of $E + E_1$ in directions orthogonal to $\vec{v}_1$ is just $(1 + o(1))\varepsilon$.

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Analogous statement for matrix power iteration is **not true.**

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- Non-orthogonal (*e.g.*, overcomplete) CP decomposition is active area of research.

Questions?

6. Tensor algebra

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- $\vec{v} \otimes \vec{w}$ (tensor product of $\vec{v} \in V$ and $\vec{w} \in W$) is the equivalence class of $E_{\vec{v},\vec{w}}$ in $V \bigotimes W$.

Tensor algebra perspective

From tensor algebra: Since $\{\vec{v}_t \;:\; t \in [n]\}$ is a basis for $\mathbb{R}^n$,
$\left\{\vec{v}_i \otimes \vec{v}_j \otimes \vec{v}_k \;:\; i, j, k \in [n]\right\}$ is a *basis* for $\mathbb{R}^n \bigotimes \mathbb{R}^n \bigotimes \mathbb{R}^n$
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Every tensor $T \in \mathbb{R}^n \bigotimes \mathbb{R}^n \bigotimes \mathbb{R}^n$ has a unique representation in this basis:

$$T = \sum_{i,j,k} c_{i,j,k} \; \vec{v}_i \otimes \vec{v}_j \otimes \vec{v}_k$$

N.B.: $\dim(\mathbb{R}^n \bigotimes \mathbb{R}^n \bigotimes \mathbb{R}^n) = n^3$.

Aside: general bases for $\mathbb{R}^n \bigotimes \mathbb{R}^n \bigotimes \mathbb{R}^n$

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Claim: A tensor T can be diagonal w.r.t. at most one basis.

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Rank-K **canonical polyadic decomposition** (CPD) of T
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N.B.: *Overcomplete* ($K > n$) CPD is also interesting *and a possibility* as long as $K(3n + 1) \ll n^3$.

7. Initialization

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Try $O(n^{1.3})$ initializers; chances are at least one is good.
(Very conservative estimate only; can be *much* better than this.)