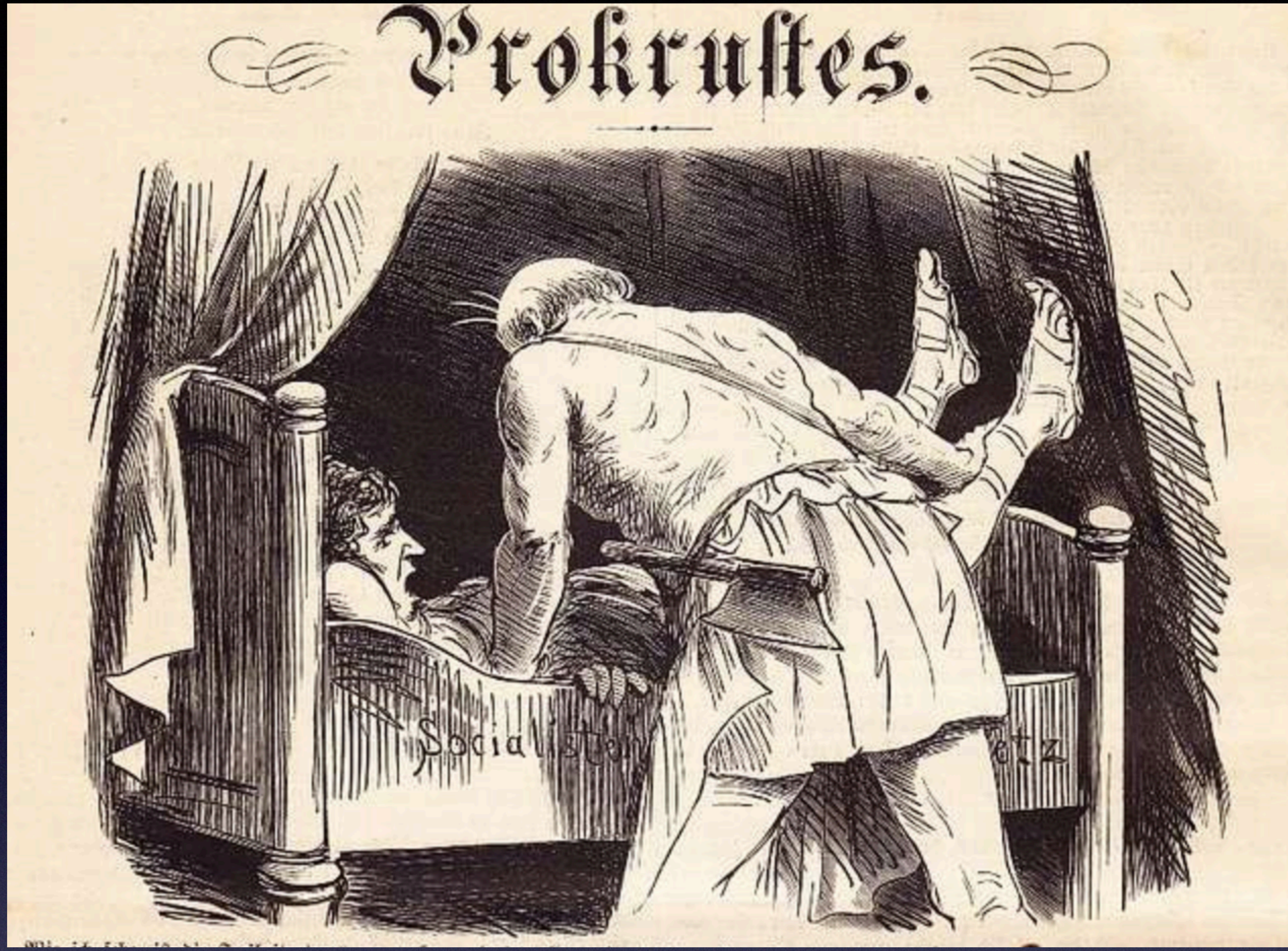
Randomized Truncation



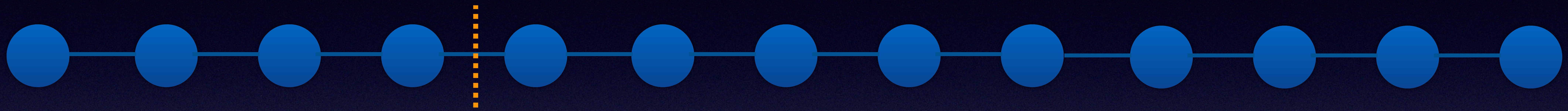
Aram Harrow
IHP Tensor workshop
15 October 2024

work in progress with
Angus Lowe & Freek Witteveen;
Minh Tran & Alexander Zlokapa

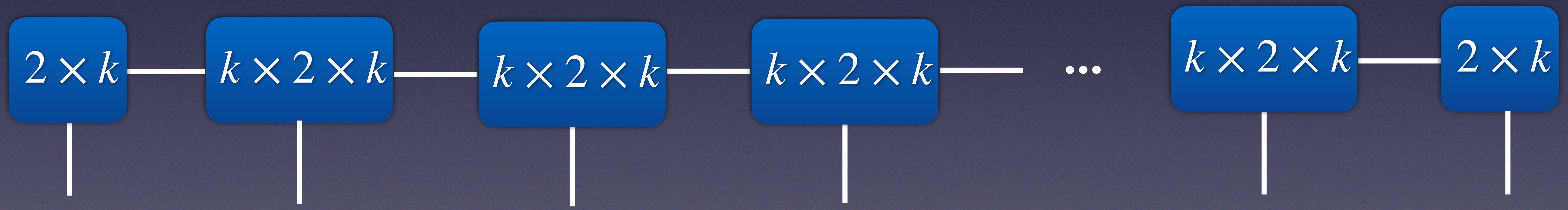
Motivation: matrix product state truncation

N qubits with state $\psi_{i_1,\ldots,i_n} \in (\mathbb{C}^2)^{\otimes n}$

rank ≤k across any cut



➡ O(Nk²) degrees of freedom suffice. k = bond dimension



$\psi_{i_1,\ldots,i_n} = \mathrm{tr}[T^{(1)}_{i_1} T^{(2)}_{i_2} \cdots T^{(n)}_{i_n}]$ with each $T^{(a)}_i \in \mathbb{C}^{k\times k}$

Given an MPS, how should we reduce its bond dimension?

A simpler problem

Given $|\psi\rangle = \sum_{i=1}^{d} v_i |i\rangle \otimes |i\rangle$ with $v_1 \geq \cdots \geq v_d \geq 0$,

what is the best approximation with Schmidt rank ≤ k?

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$$|\varphi\rangle \propto \sum_{i=1}^{k} v_i |i\rangle \otimes |i\rangle \qquad F = \sqrt{\sum_{i=1}^{k} v_i^2}$$

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<u>Fidelity</u>

$$F(\rho, \sigma) = \left\| \sqrt{\rho}\sqrt{\sigma} \right\|_1$$

$$= |\langle v | w \rangle|$$

for pure states

An even simpler problem

Given $|v\rangle = \sum_{i=1}^{d} v_i |i\rangle$ with $v_1 \geq \cdots \geq v_d \geq 0$,

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$$|w\rangle = F^{-1} \sum_{i=1}^{k} v_i |i\rangle \qquad F = \sqrt{\sum_{i=1}^{k} v_i^2}$$

Fidelity

$$F(\rho, \sigma) = \left\| \sqrt{\rho}\sqrt{\sigma} \right\|_1$$

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What about other metrics?

Given $|v\rangle = \sum_{i=1}^{d} v_i |i\rangle$ with $v_1 \geq \cdots \geq v_d \geq 0$, find a close k-sparse $|w\rangle$.

Metric	Definition	Optimum
F fidelity	$\lvert\langle v \vert w \rangle\rvert$	$\sqrt{\sum_{i=1}^{k} v_i^2}$
T trace distance	$\frac{1}{2} \lVert\, \lvert v\rangle\langle v\rvert - \lvert w\rangle\langle w\rvert \,\rVert_1$	$F^2 + T^2 = 1$ for pure states
D relative entropy	$\langle v\vert$ -ln σ $\vert v\rangle$	0 or ∞
D_{max} = ln(1+R) D_{max} = max-relative entropy R = robustness	min{λ: $\vert v\rangle\langle v\vert \leq e^{\lambda}\sigma$}	0 or ∞

with Angus Lowe and Freek Witteveen

Mixed-state approximations

Given $|v\rangle = \sum_{i=1}^{d} v_i|i\rangle$ find a nearby σ, a mixture of k-sparse states.

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T trace distance	$\frac{1}{2} \Vert \, \vert v\rangle\langle v \vert - \sigma \, \Vert_1$	$\sqrt{\epsilon}$	$\frac{\epsilon}{2} \lessapprox T \leq \sqrt{\epsilon}$

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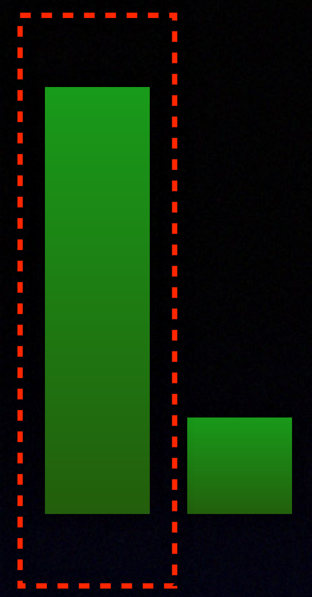
D relative entropy	⟨v| -ln σ |v⟩	0 or ∞	?
R robustness	min{R: |v⟩⟨v| ≤(1+R)σ}	0 or ∞	later

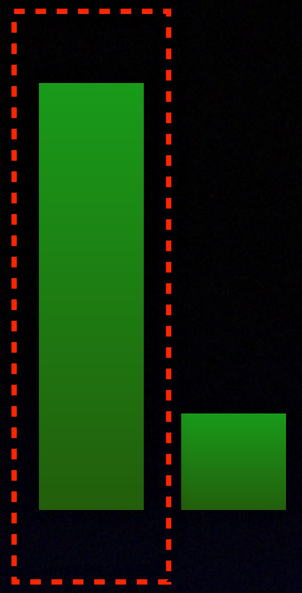
Example 1



$$|v\rangle = \sqrt{1-\epsilon}\,|0\rangle + \sqrt{\epsilon}\,|1\rangle$$

$$|v\rangle\langle v| = \begin{pmatrix} 1-\epsilon & \sqrt{\epsilon(1-\epsilon)} \\ \sqrt{\epsilon(1-\epsilon)} & \epsilon \end{pmatrix}$$

k=1



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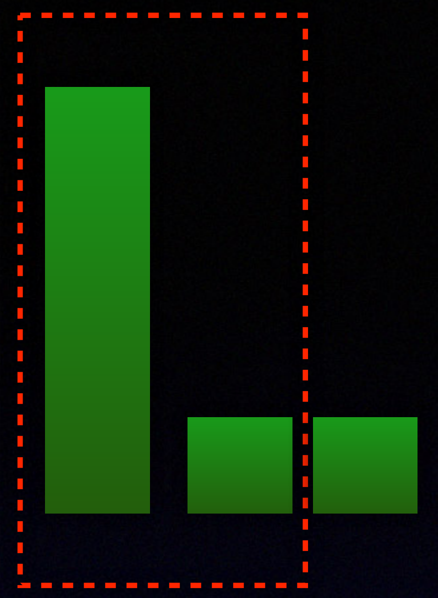
k=1

Best 1-sparse approximation

	σ	F	T	R
Pure	$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$	$\sqrt{1-\epsilon}$	$\sqrt{\epsilon}$	∞
Mixed	$\begin{pmatrix} 1-\epsilon & 0 \\ 0 & \epsilon \end{pmatrix}$	$\sqrt{1-2\epsilon+2\epsilon^2}$	$\sqrt{\epsilon-\epsilon^2}$	$2\sqrt{\epsilon-\epsilon^2}$

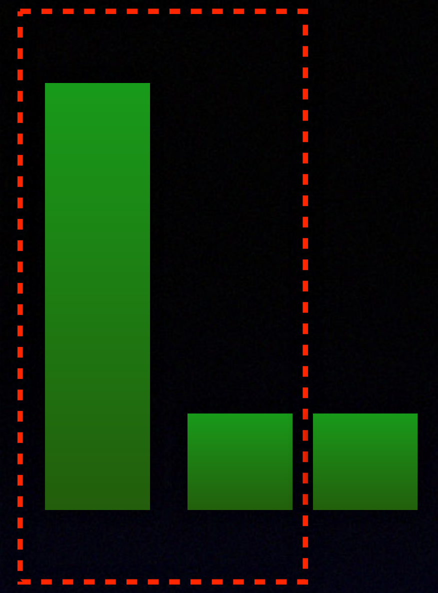
Example 2



$$|v\rangle = \sqrt{1-2\epsilon}\,|0\rangle + \sqrt{\epsilon}\,|1\rangle + \sqrt{\epsilon}\,|2\rangle$$

k=2

$$|v\rangle\langle v| = \begin{pmatrix} 1-2\epsilon & \sqrt{\epsilon(1-2\epsilon)} & \sqrt{\epsilon(1-2\epsilon)} \\ \sqrt{\epsilon(1-2\epsilon)} & \epsilon & \epsilon \\ \sqrt{\epsilon(1-2\epsilon)} & \epsilon & \epsilon \end{pmatrix}$$



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k=2

Best 2-sparse approximation

	σ	F	T	R
Pure	$\propto \begin{pmatrix} 1-2\epsilon & \sqrt{\epsilon(1-2\epsilon)} & 0 \\ \sqrt{\epsilon(1-2\epsilon)} & \epsilon & 0 \\ 0 & 0 & 0 \end{pmatrix}$	$\sqrt{1-\epsilon}$	$\sqrt{\epsilon}$	∞
Mixed	$\sqrt{1-4\epsilon}\,|0\rangle$ $+\sqrt{4\epsilon}\,|1 \text{ or } 2\rangle$	≈1-ε	O(ε)	2ε

Example 3

$$|v\rangle = \sqrt{\frac{1}{d}}\sum_{i=1}^{d}|i\rangle$$

k=d(1-ε)

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$$|v\rangle = \sqrt{\frac{1}{d}} \sum_{i=1}^{d} |i\rangle$$

k=d(1-ε)

Best k-sparse approximation

	σ	F	T	R
Pure	$|S\rangle = \sqrt{\frac{1}{k}} \sum_{i \in S} |i\rangle$	$\sqrt{1-\epsilon}$	$\sqrt{\epsilon}$	∞
Mixed	$\mathbb{E}\,|S\rangle\langle S|$	$\sqrt{1-\epsilon}$	≈ε	$\frac{\epsilon}{1-\epsilon}$

Example 4

$$|v\rangle = \sqrt{\frac{1-\epsilon}{k}} \sum_{i=1}^{k} |i\rangle + \sqrt{\frac{\epsilon}{d}} \sum_{i=k+1}^{d+k} |i\rangle$$

d ≫ k, dkε > 1

Example 4

$$|v\rangle = \sqrt{\frac{1-\epsilon}{k}} \sum_{i=1}^{k} |i\rangle + \sqrt{\frac{\epsilon}{d}} \sum_{i=k+1}^{d+k} |i\rangle$$

$d \gg k$, $dk\varepsilon > 1$

Best k-sparse approximation

	σ	F	T	R
Pure	$\sqrt{\frac{1}{k}} \sum_{i=1}^{k} \|i\rangle$	$\sqrt{1-\epsilon}$	$\sqrt{\epsilon}$	∞
Mixed	$\sqrt{\frac{1}{k}} \sum_{i=1}^{k} \|i\rangle$	$\sqrt{1-\epsilon}$	$\sqrt{\epsilon}$	$d\varepsilon$ or $d\varepsilon/k$

Finding optimal approximations

k-incoherent states

$I_k = \mathrm{conv}\{|w\rangle\langle w| : |w\rangle \text{ is k-sparse}\}$

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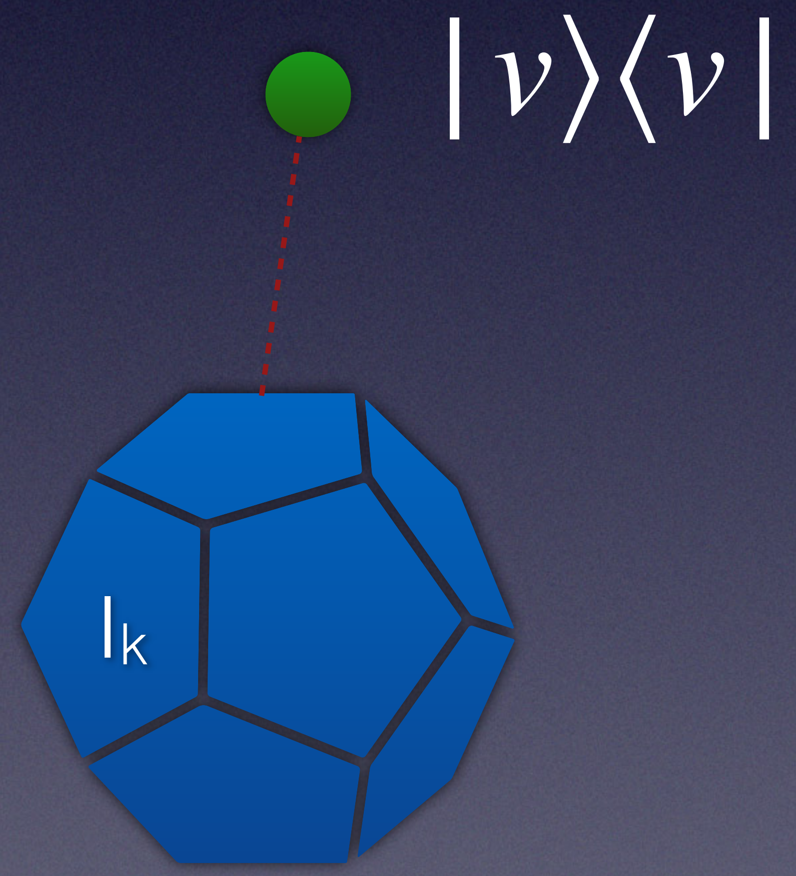

Goals

- $\max F(|v\rangle\langle v|, \sigma)$
- $\min \| \, |v\rangle\langle v| - \sigma \, \|_1$
- $\min D(|v\rangle\langle v| \, \| \, \sigma)$
- $\min R$ s.t. $|v\rangle\langle v| \leq (1+R)\sigma$

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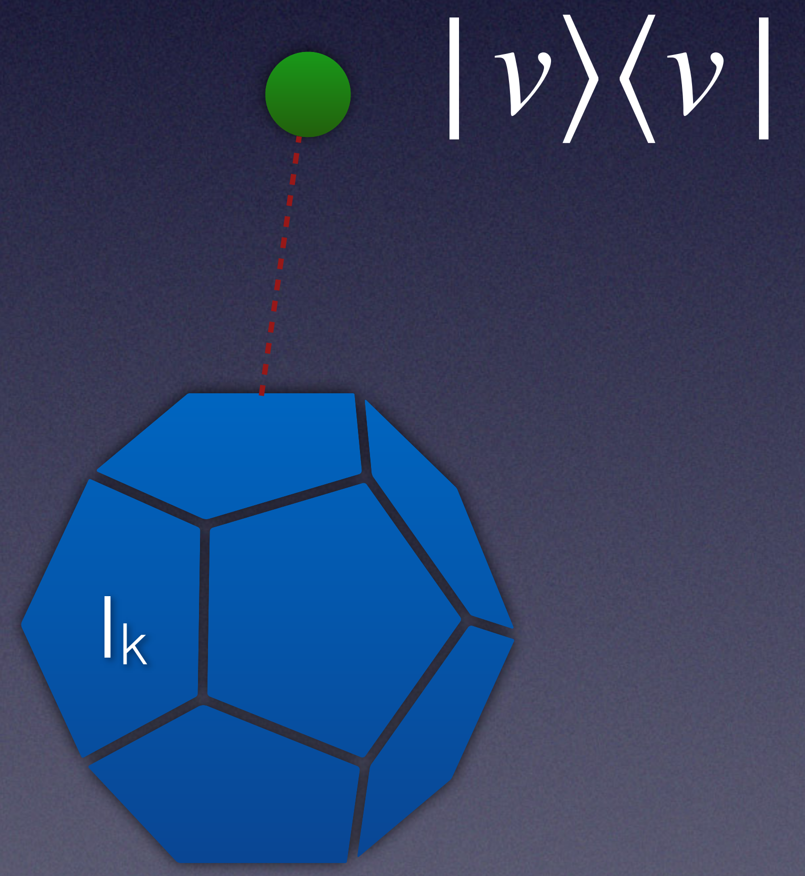

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However, it's NP-complete to

- Test membership in I_k.
- Optimize linear functions over I_k.
- Can "brute-force" in time $d^{O(k)}$

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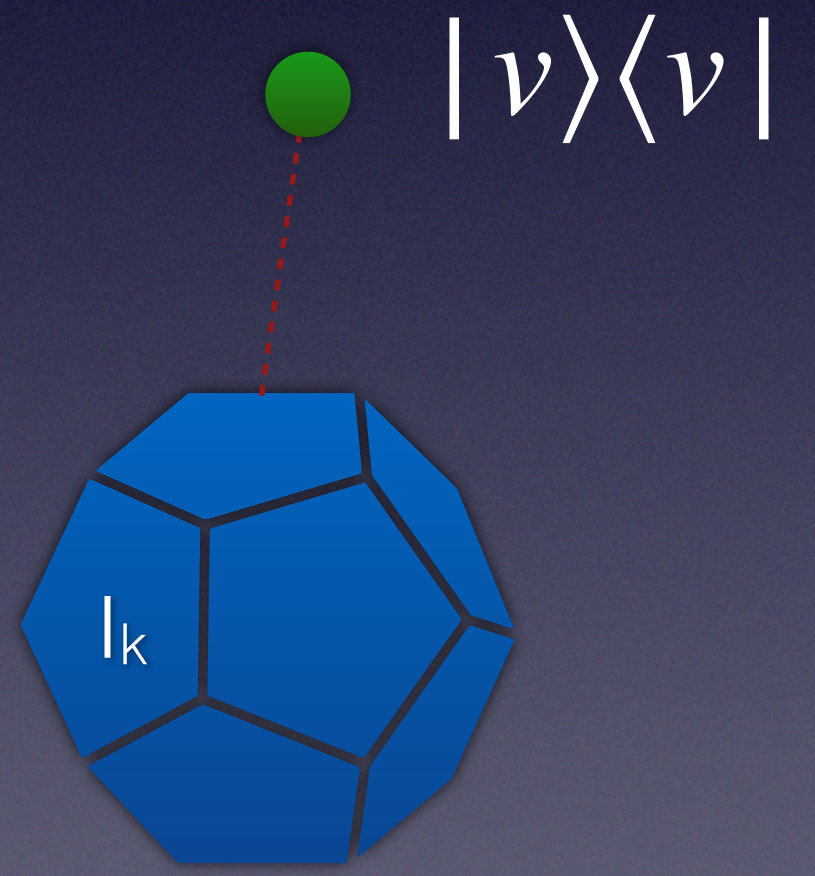

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A = adjacency matrix of a graph
$\max \{\text{tr } A\sigma : \sigma \in I_k\} = k-1$ iff A has a k-clique

The k-support norm

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Top-k norm

$$\|v\|_{(k)} := \sqrt{\sum_{i=1}^{k} |v_i^{\downarrow}|^2}$$

Assuming $v_1 \geq v_2 \geq \ldots$

$$\|v\|_{(k)}^2 := \sum_{i=1}^{k} v_i^2$$

$F = \|v\|_{(k)}$

The k-support norm

[Agyriou, Foygel, Srebro. NeurIPS 2012]

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k-support norm

$$\|v\|_{(k,*)} = \max_{\|w\|_{(k)} \leq 1} \langle v, w \rangle$$

$$= \min \left\{ \sum_{\alpha} \|w_\alpha\|_2 : v = \sum_{\alpha} w_\alpha, \|w_\alpha\|_0 \leq k \right\}$$

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$$\|v\|_\infty \leq \|v\|_{(k)} \leq \|v\|_2 \leq \|v\|_{(k,*)} \leq \|v\|_1$$

$$1 + R = \|v\|_{(k,*)}^2$$

[Johnston, Li, Plosker, Poon, Regula. PRA 2018; Regula. J. Phys. A 2018]

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Robustness / D_{max}

see also [Ferris, 1507.00767]

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$$\|v\|_{(k,*)} = \max_{\|w\|_{(k)}\leq 1} \langle v, w \rangle$$

$$1 + R = \|v\|^2_{(k,*)} = \sum_{i=1}^{k-r-1} v_i^2 + \frac{s_{k-r}^2}{r+1}$$

where r is chosen so that

$$v_{k-r-1} > \frac{s_{k-r}}{r+1} \geq v_{k-r}$$

and $s_{k-r} = \sum_{i \geq k-r} v_i$

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and $s_{k-r} = \sum_{i\geq k-r} v_i$

Ensemble construction

$$\frac{(v_1, \ldots, v_{k-r-1}, 0, \alpha, \alpha, 0, \alpha, 0, 0, 0, \alpha, \ldots)}{\|v\|_{(k,*)}}$$

where $\alpha = \dfrac{s_{k-r}}{r+1}$ appears in entry i with probability $\dfrac{v_i}{\alpha}$

see also [Ferris, 1507.00767]

Trace distance

$$T = \min_{\sigma \in I_k} \frac{1}{2} \| vv^* - \sigma \|_1$$

$$= \min_{\sigma \in I_k} \max_{0 \le M \le I} \mathrm{tr}[M(vv^* - \sigma)]$$

$$= \min_{\sigma \in I_k} \max_{\|m\|_2 \le 1} \mathrm{tr}[mm^*(vv^* - \sigma)]$$ $vv^* - \sigma$ has one positive evalue

$$= \min_{\sigma \in I_k} \max_{\|\rho\|_{S_1} \le 1} \mathrm{tr}[\rho(vv^* - \sigma)]$$ convexify

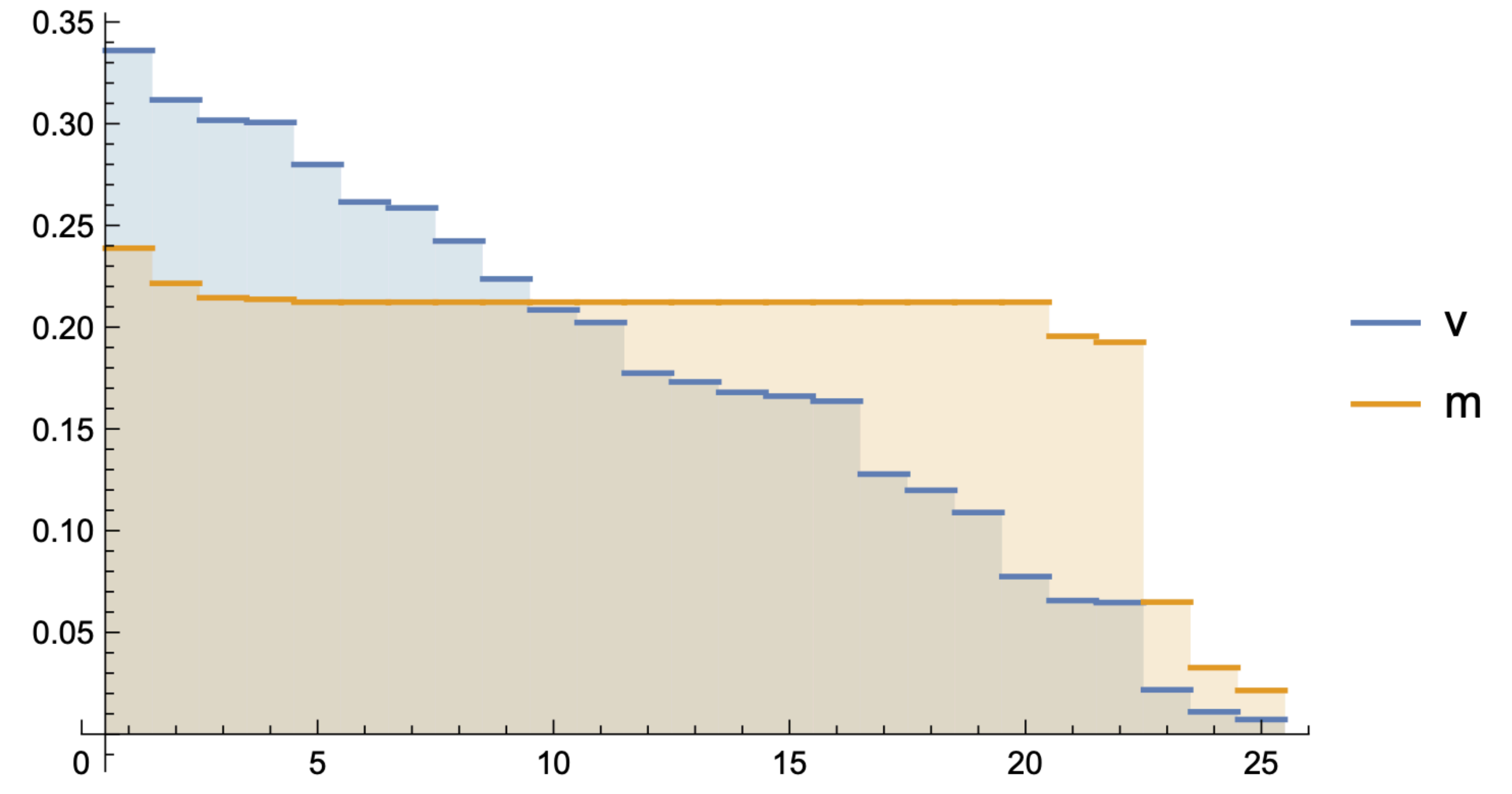
$$= \max_{\|\rho\|_{S_1} \le 1} \min_{\sigma \in I_k} \mathrm{tr}[\rho(vv^* - \sigma)]$$ minimax

$$= \max_{\|m\|_2 \le 1} \min_{\sigma \in I_k} \mathrm{tr}[mm^*(vv^* - \sigma)]$$

$$= \max_{\|m\|_2 \le 1} |\langle m | v \rangle|^2 - \|m\|_{(k,*)}^2$$

Trace distance via dual

$$T = \min_{\sigma \in I_k} \frac{1}{2} \| \, |v\rangle\langle v| - \sigma \, \|_1 = \max_{\|m\|_2 \le 1} |\langle m | v \rangle|^2 - \|m\|^2_{(k),*}$$



Optimal measurement is $|m\rangle\langle m|$.

Find m using Lagrange multipliers

Sample from

$$m_i \propto \begin{cases} \frac{v_i}{1+\lambda} & 1 \le i < k-r \\ \theta & k-r \le i < \ell \\ \frac{v_i}{\lambda} & \ell < i \end{cases}$$

$$\varphi \propto \begin{cases} v_1, \ldots, v_{k-r-1} & \\ \alpha,0,0,\alpha,0 & k-r \le i < \ell \\ 0,0,\ldots & \ell \le i \end{cases}$$

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D relative entropy	⟨v| -ln σ |v⟩	0 or ∞	$\varepsilon \leq D \leq D_{max}$
$D_{max} = \ln(1+R)$	$\min\{\lambda: |v\rangle\langle v| \leq e^{\lambda}\sigma\}$	0 or ∞	$1 + R = \|v\|^2_{(k,*)}$

Application: Hamiltonian simulation

Goal: e^{-iHt} for $H = \sum_{j=1}^{L} \beta_j h_j$ with $\|h_j\| = 1$ and $\sum_j \beta_j = 1$.

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Trotter: $\left(e^{-i\beta_1 h_1 \delta} e^{-i\beta_2 h_2 \delta} \ldots e^{-i\beta_L h_L \delta}\right)^{t/\delta}$

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qDRIFT: Apply $e^{-i\delta h_j}$ with probability β_j. Repeat t/δ times.

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Mixed low-rank approximation: To first order in t,

$|\psi\rangle - it \sum_{j=1}^{L} \beta_j h_j |\psi\rangle \approx$ mixture of states of the form $\propto |\psi\rangle - ith_j|\psi\rangle$.

randomized H simulation

$$H = \sum_{j=1}^{L} \beta_j h_j \text{ with } \|h_j\| = 1, \ \sum_j \beta_j = 1 \text{ and } \beta_1 \geq \beta_2 \geq \cdots$$

General framework:

- Randomize: Evolve according to $H(u) = \sum_j u_j h_j$ with probability p_u.
- Unbiased (to first order): $\sum_u p_u u = \beta$
- Optimize variance and second-order bias: $\|\beta\beta^T - \sum_u p_u u u^T\|_{\text{various}}$

Previous work: SparSto [Ouyang, White, Campbell. 2020] Partially random Trotter [Jin, Li. 2021] composite qDRIFT [Hagan, Wiebe. 2022] and [Pocrnic, Hagan, Carrasquilla, Segal, Wiebe. 2023]

state-dependent simulation

$H = \sum_{j=1}^{L} \beta_j h_j$ with $||h_j|| = 1$, applied to state $|\psi\rangle$

First-order condition: $\sum_j (\beta_j - \sum_u p_u u_j) h_j |\psi\rangle = 0$

Second-order error terms: $||\beta\beta^T - \sum_u p_u u u^T||_{\text{state dept.}}$

- maximally mixed marginals —> each $h_j |\psi\rangle$ is orthogonal
- low-frustration states —> smaller norm

Data needed

$\langle\psi| h_i h_j |\psi\rangle$

Classical vectors

- Approximate v with a random k-sparse w.
- $v = \mathbb{E}[w]$
- minimize $\|vv^* - \mathbb{E}[ww^*]\|_\infty = \epsilon$
- If $f(v) = \langle m, v \rangle$ then $\epsilon = \max_m \text{Var}[f(w) - f(v)]$
- Same trace-distance construction works for $\| \cdot \|_\infty$