Quantum gradient estimation and its application to quantum reinforcement learning

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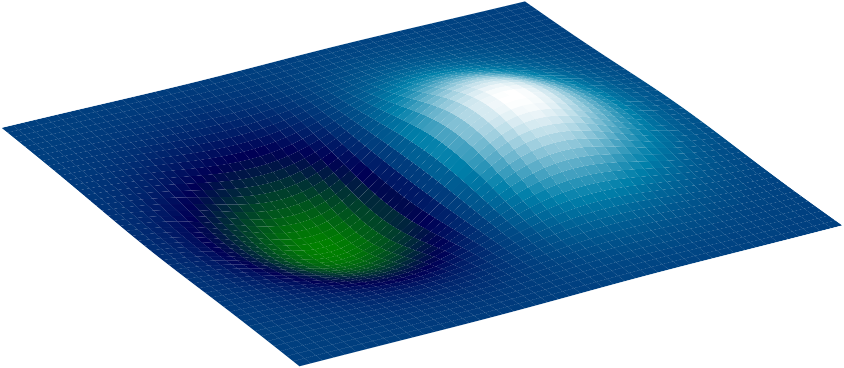

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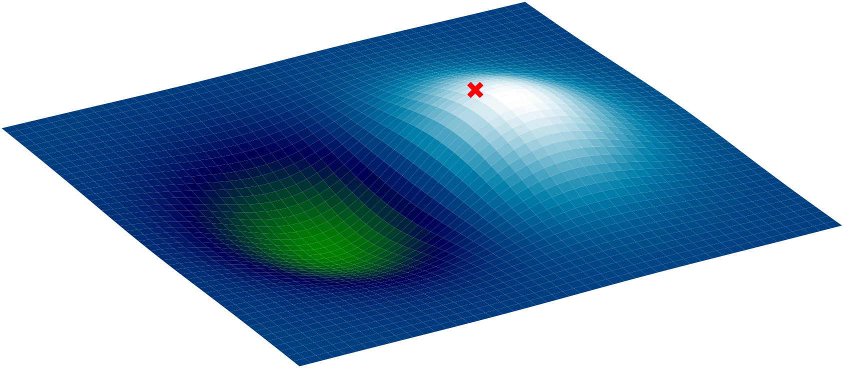

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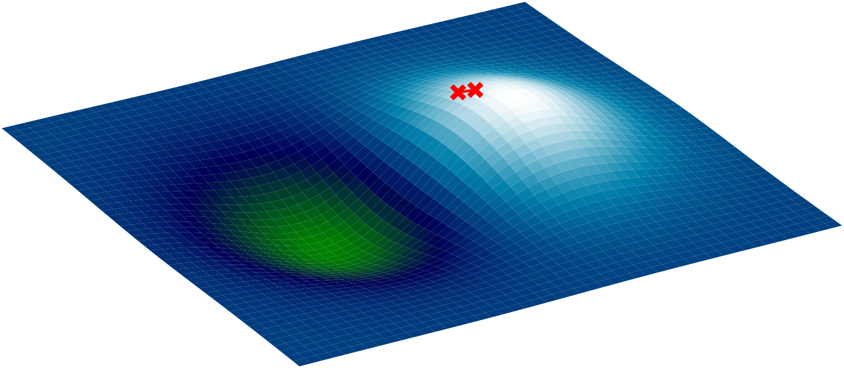

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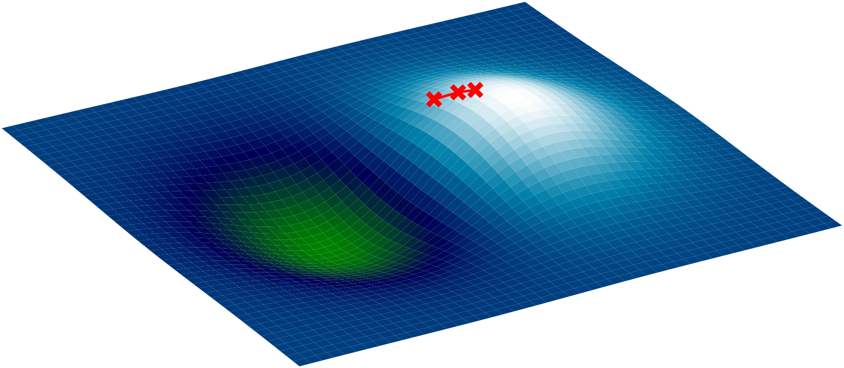

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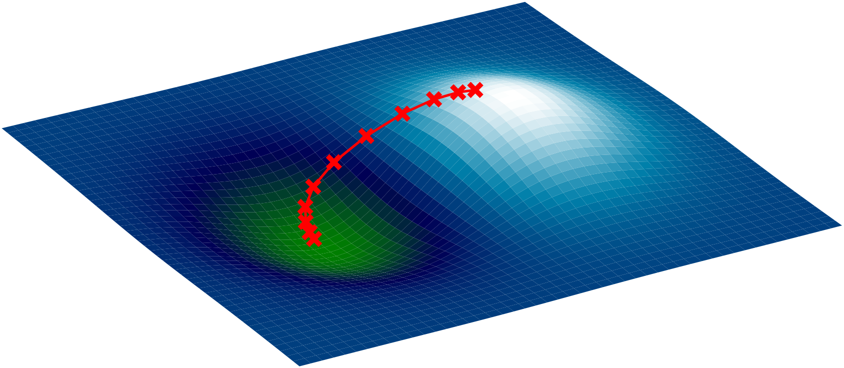

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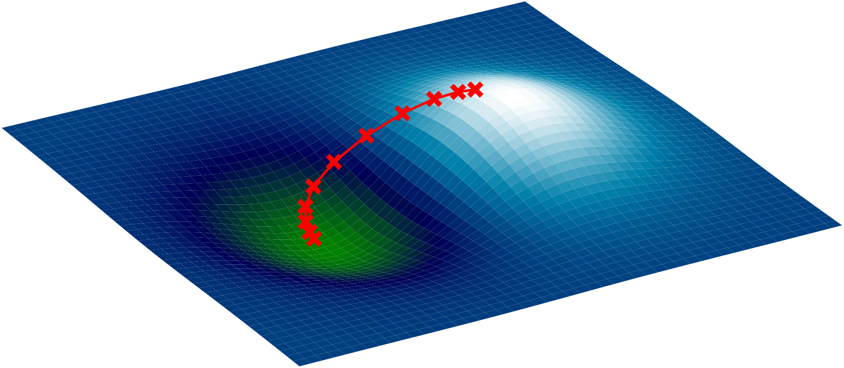

Can we speed up the gradient calculation step when d is large?

Classical gradient estimation

Classical gradient estimation

- Easiest case: let $f : \mathbb{R}^d \to \mathbb{R}$ be linear.

$$f(\mathbf{x}) = a + g_1 x_1 + \cdots + g_d x_d, \qquad \nabla f = \begin{bmatrix} g_1 \\ \vdots \\ g_d \end{bmatrix}$$

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- **Can we do better with a quantum computer?**

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- An n-qubit state $|\psi\rangle$ is a unit vector in $\mathbb{C}^{2^n}$:

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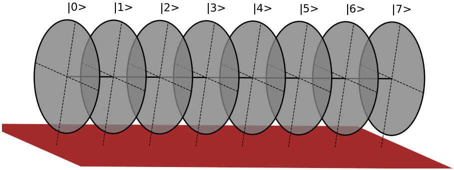

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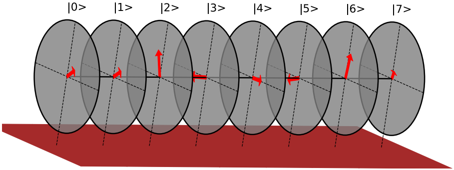

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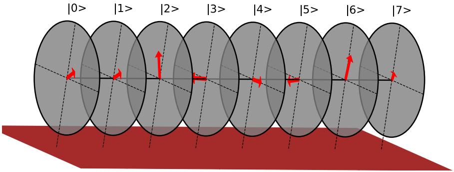

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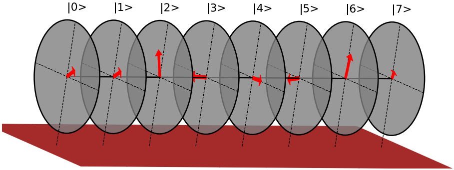

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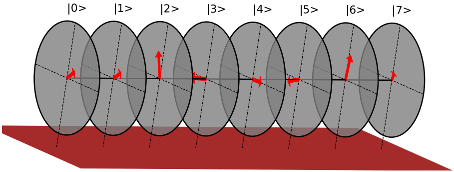

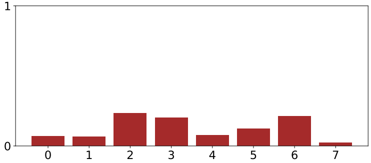

Quantum Fourier transform

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$$\mathrm{QFT}_{2^n} : |j\rangle \mapsto \frac{1}{\sqrt{2^n}} \sum_{k=0}^{2^n-1} e^{\frac{2\pi ijk}{2^n}} |k\rangle$$

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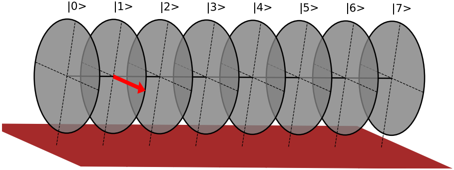

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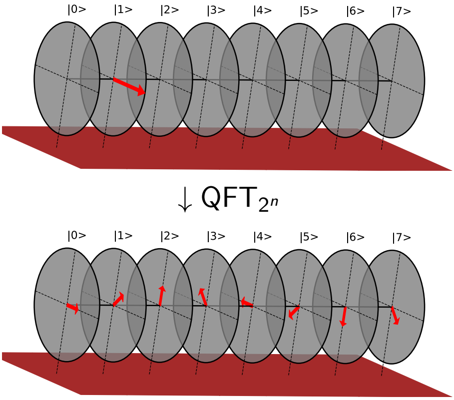

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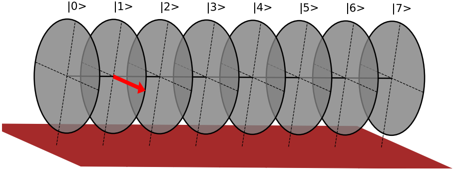

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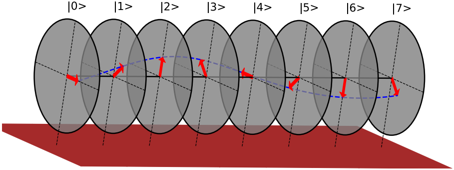

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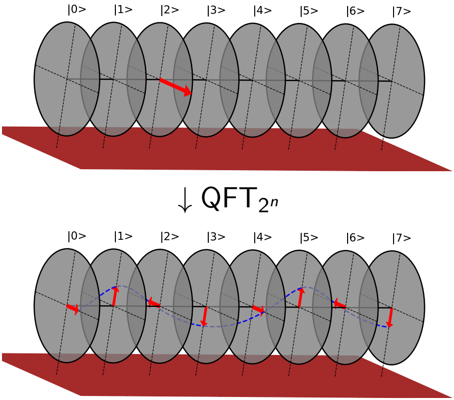

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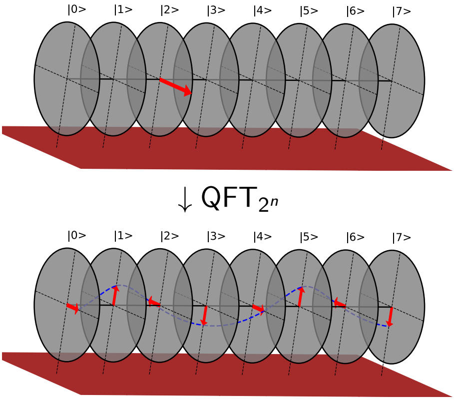

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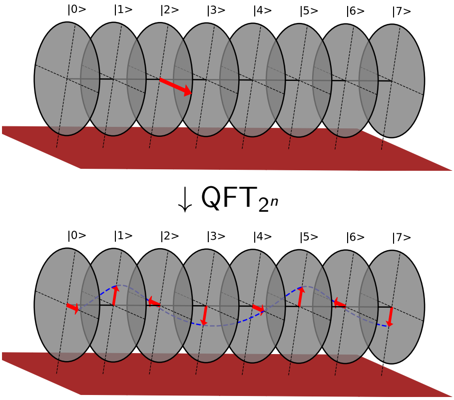

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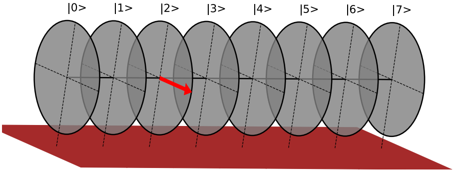

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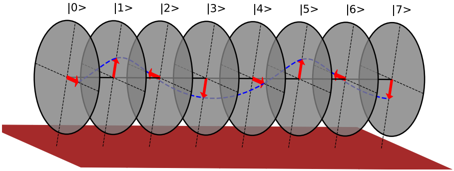

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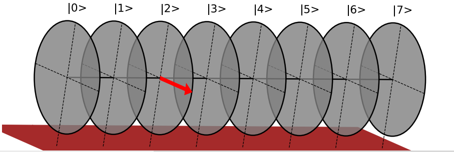

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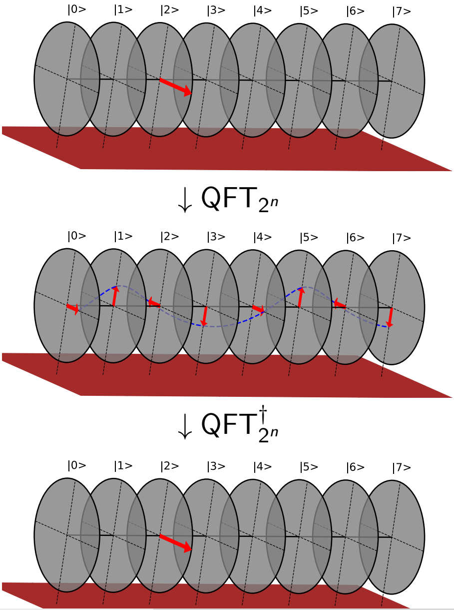

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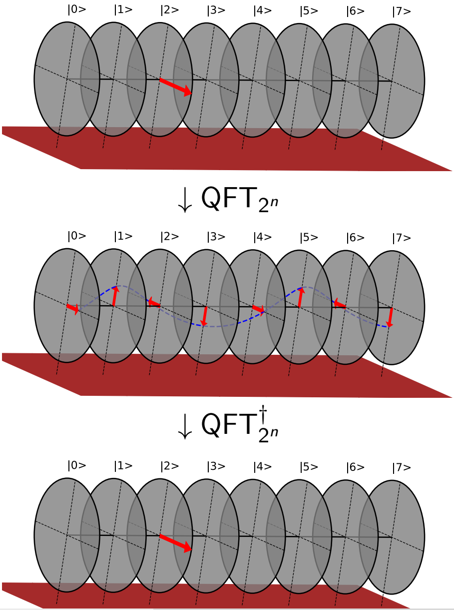

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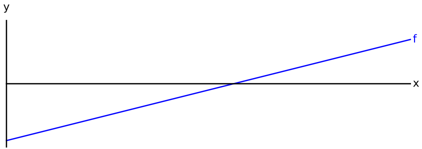

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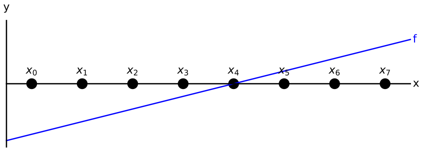

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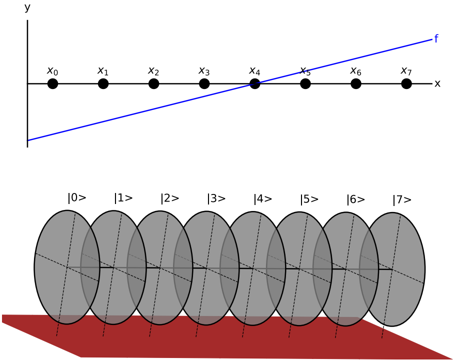

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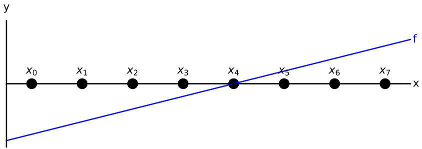

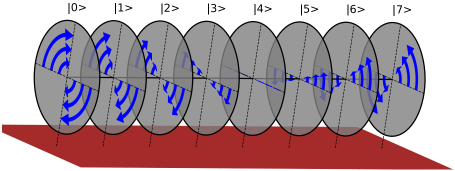

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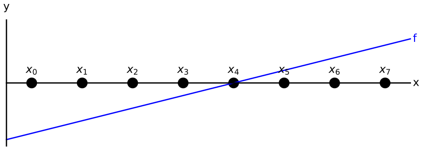

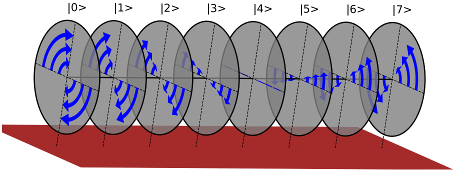

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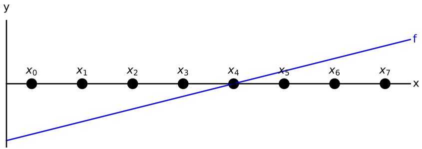
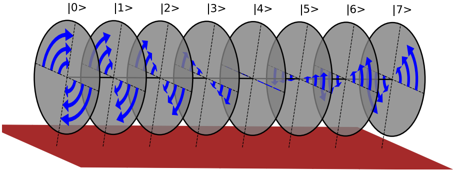
- One application of this phase oracle is one *quantum function evaluation*.





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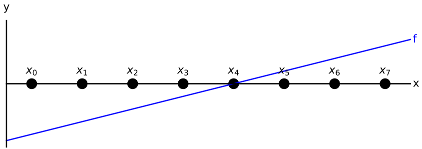

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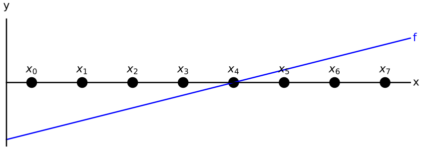

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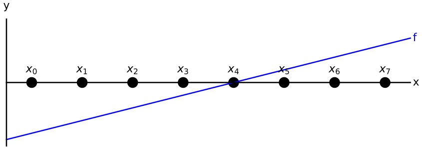

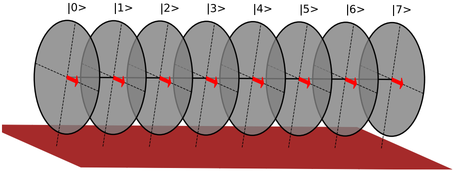

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1. Create a uniform superposition over the grid.
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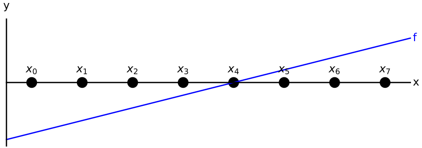

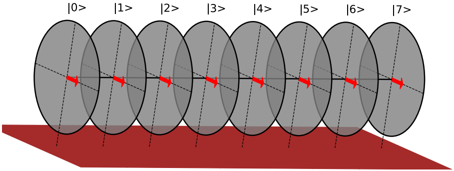

Quantum derivative estimation algorithm for linear functions

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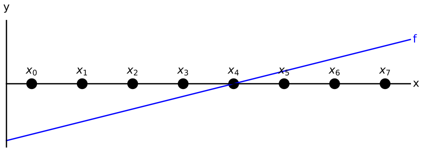

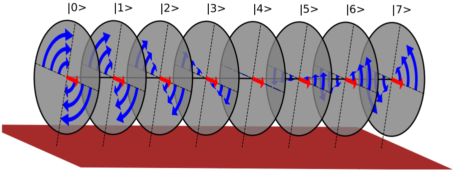

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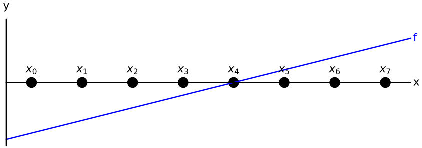

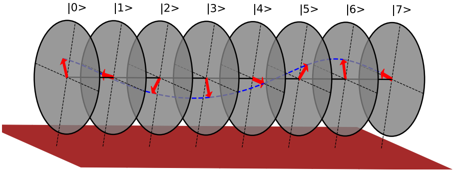

Quantum derivative estimation algorithm for linear functions

Let $f : \mathbb{R} \to \mathbb{R}$ linear with $|f'| \leq C$.

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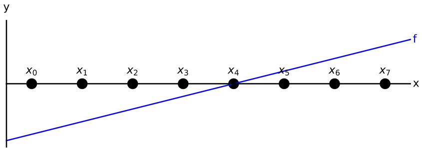
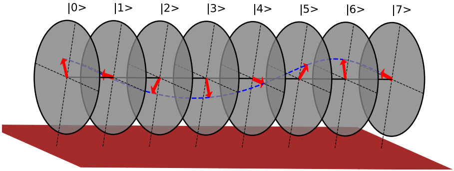
4. Measure.





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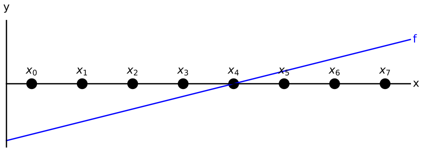

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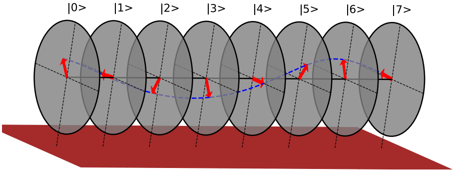

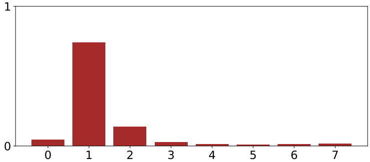

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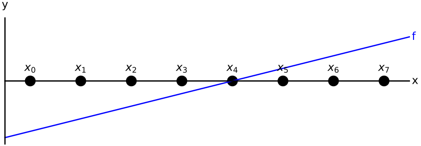
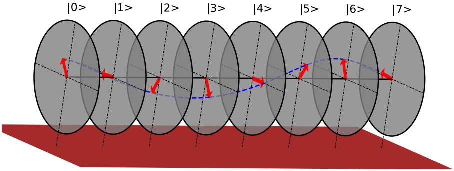
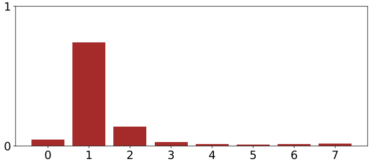
Generalizes to $f : \mathbb{R}^d \to \mathbb{R}$.
(Jordan, 2004)







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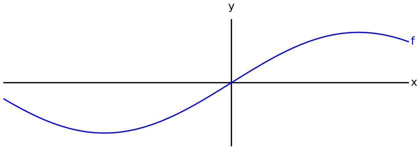

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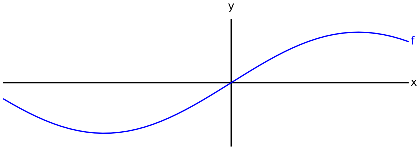

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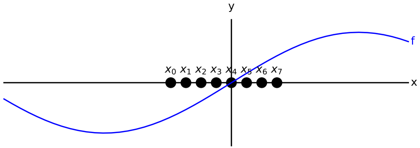

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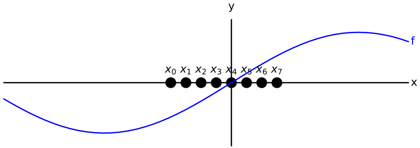

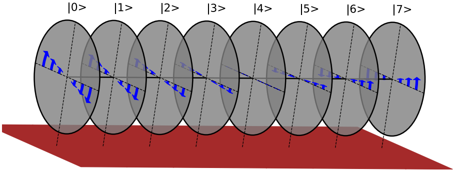

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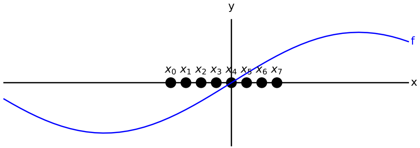

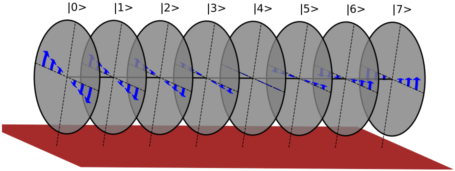

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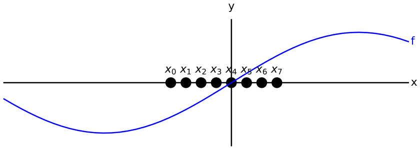

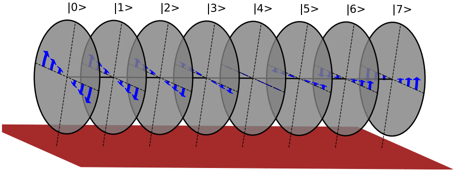

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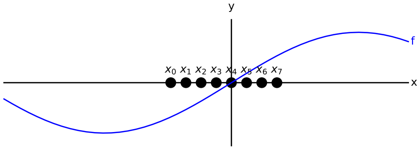

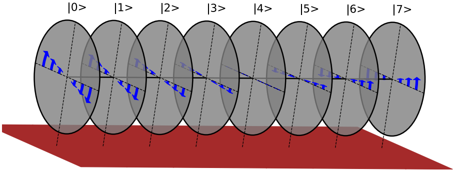

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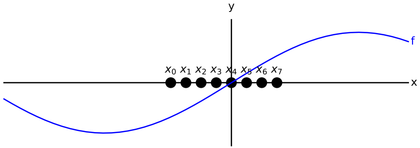
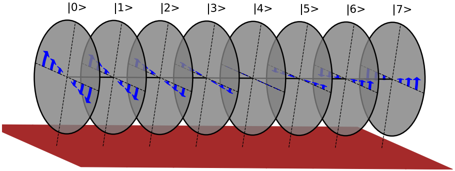
- Key idea: central difference method to extend region of approximate linearity.





Central difference method

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- Let $f : \mathbb{R}^d \to \mathbb{R}$ and $m > 0$. We define:

$$\widetilde{f}_{(2m)}(\mathbf{x}) = \sum_{\ell=-m}^{m} a_\ell^{(2m)} f(\ell\mathbf{x})$$

- such that:

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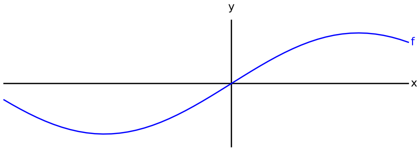

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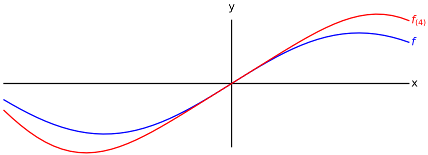

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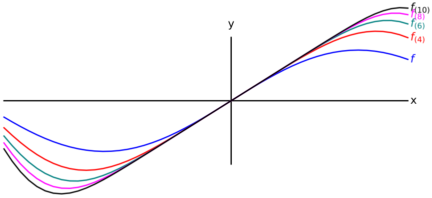

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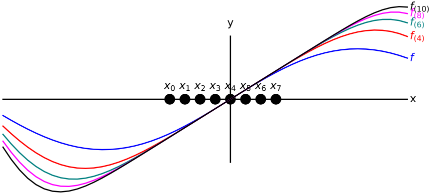

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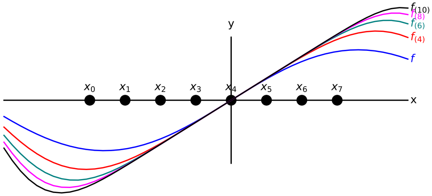

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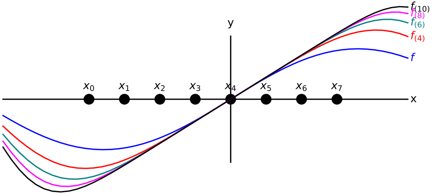

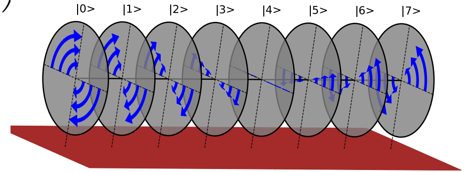

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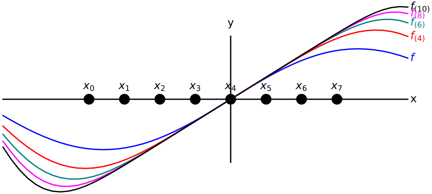
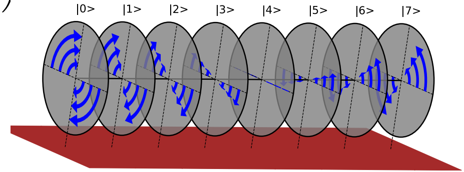
- One can implement $O_{\widetilde{f}_{(2m)}}$ using $\widetilde{\mathcal{O}}(m)$ queries to O_f. (Gilyén, Arunachalam, Wiebe, 2018)





Smoothness conditions (Gilyén et al. 2018)

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- Then $\widetilde{f}_{(k)}$ is linear.
- So gradient estimation takes $\widetilde{\mathcal{O}}(k)$ queries.

Case 2: Gevrey

- Let $f : \mathbb{R}^d \to \mathbb{R}$ have a convergent Taylor series:

$$f(\mathbf{x}) = \sum_{k=0}^{\infty} \sum_{\alpha \in [d]^k} \frac{\partial_\alpha f(\mathbf{0})}{k!} \mathbf{x}^\alpha$$

- Let $\sigma \in [\frac{1}{2}, 1]$:

$$|\partial_\alpha f(\mathbf{0})| \leq (k!)^\sigma$$

Smoothness condition	Polynomial degree k	Gevrey $\sigma \in [0, \frac{1}{2})$	Gevrey $\sigma = \frac{1}{2}$	Gevrey $\sigma \in (\frac{1}{2}, 1]$
Best known algorithm	$\widetilde{\mathcal{O}}(k)$	$\widetilde{\mathcal{O}}(d^{\frac{1}{2}})$	$\widetilde{\mathcal{O}}(d^{\frac{1}{2}})$	$\widetilde{\mathcal{O}}(d^{\sigma})$
Best known lower bound	$\Omega(1)$	$\Omega(d^{\frac{1}{2}})$	$\Omega(d^{\frac{1}{2}})$	$\Omega(d^{\frac{1}{2}})$

Smoothness conditions (Gilyén et al. 2018)

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From ℓ^∞ to ℓ^p approximations: multiply upper and lower bounds by $\Theta(d^{\frac{1}{p}})$.

Analog arithmetics (Gilyén et al., 2018)

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Probability oracle
$$U_f : |\mathbf{x}\rangle |0\rangle \mapsto |\mathbf{x}\rangle \left(\sqrt{f(\mathbf{x})}\,|1\rangle + \sqrt{1 - f(\mathbf{x})}\,|0\rangle\right)$$

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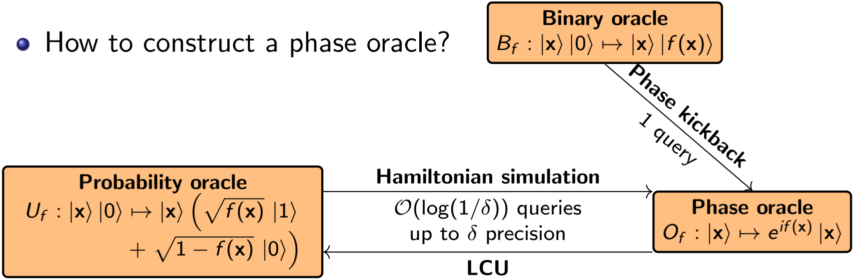

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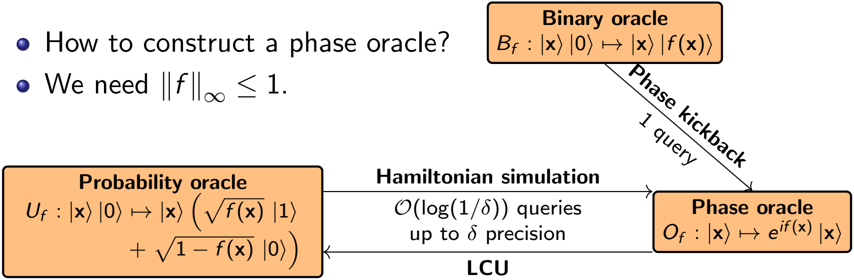

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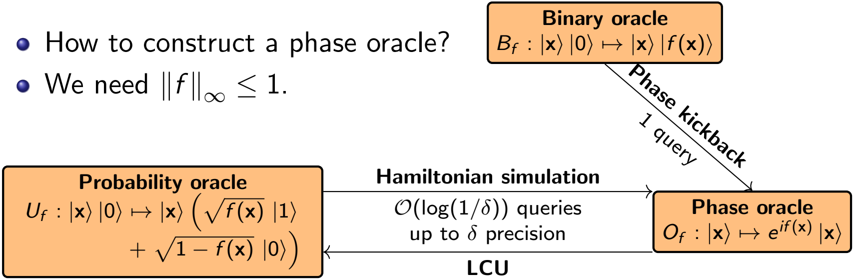

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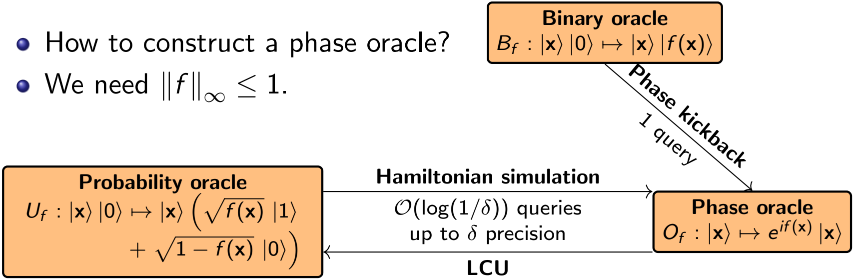

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Hamiltonian simulation
$\mathcal{O}(\log(1/\delta))$ queries
up to δ precision
LCU

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  - **Multiplication:** consecutive applications of probabilty oracles.

$$(U_f)_1 (U_g)_2 : |\mathbf{x}\rangle |00\rangle \mapsto \sqrt{f(\mathbf{x}) g(\mathbf{x})}\, |\mathbf{x}\rangle |11\rangle + |\perp\rangle$$

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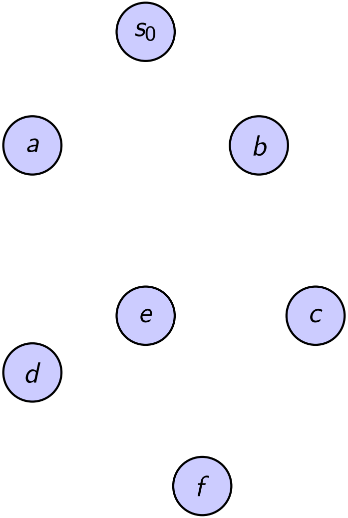

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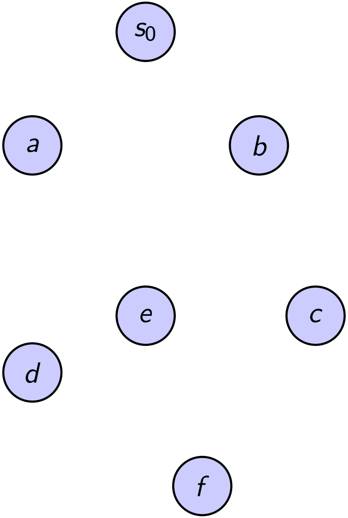

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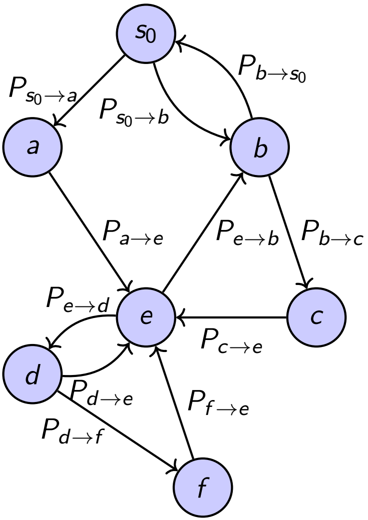

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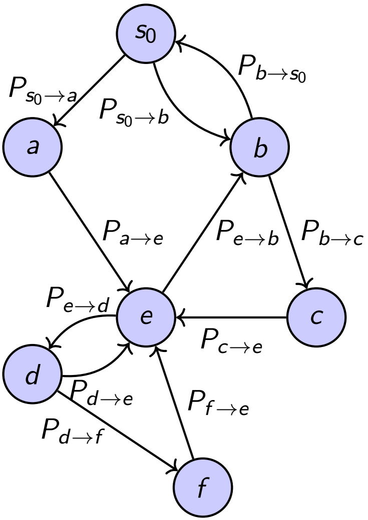

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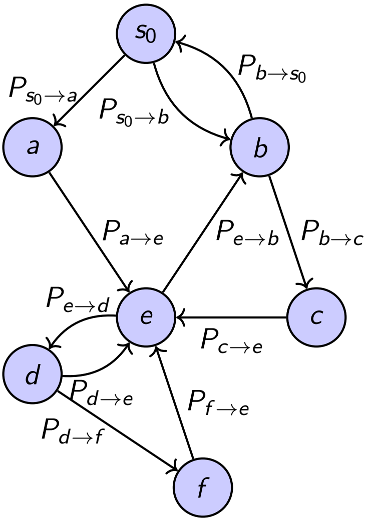

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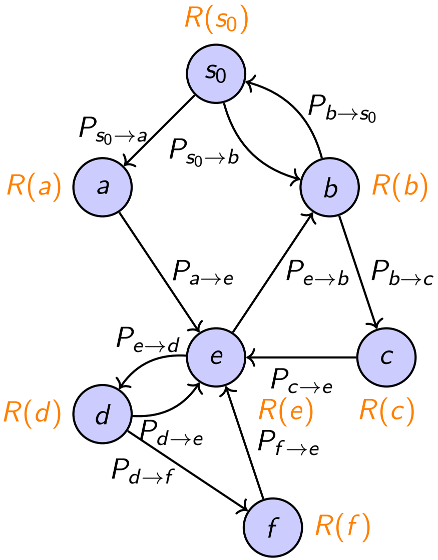

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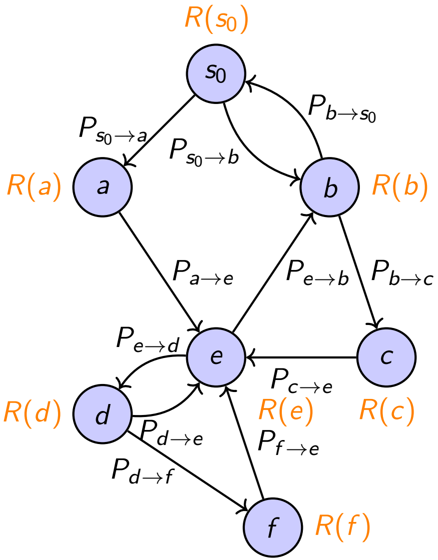

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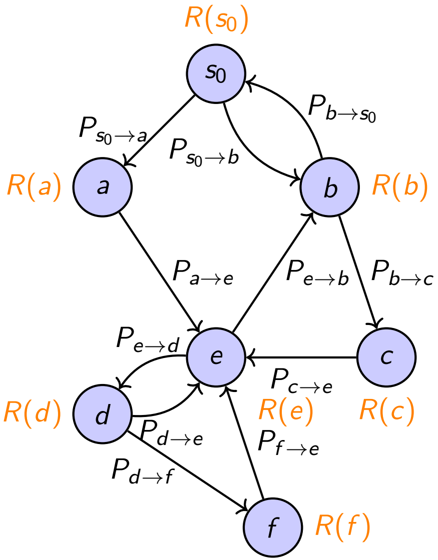

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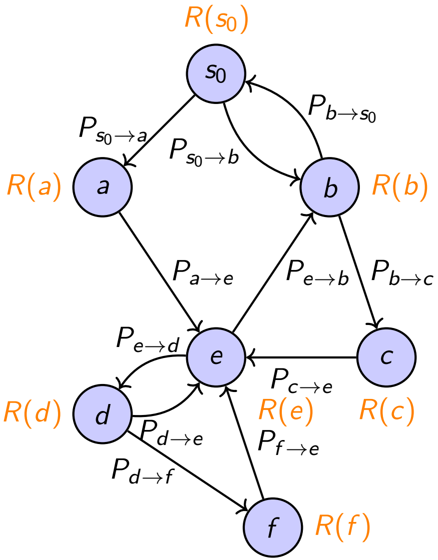

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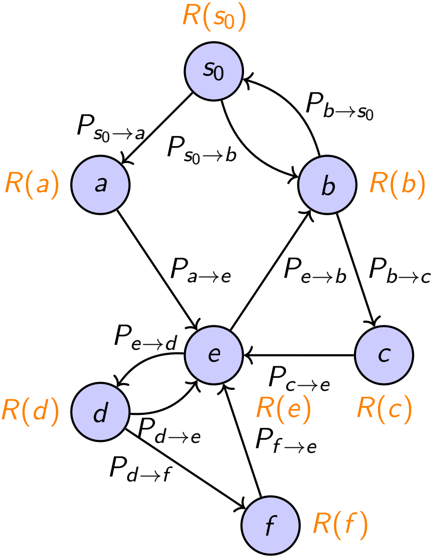

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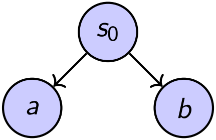

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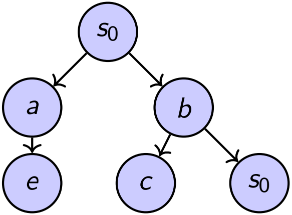

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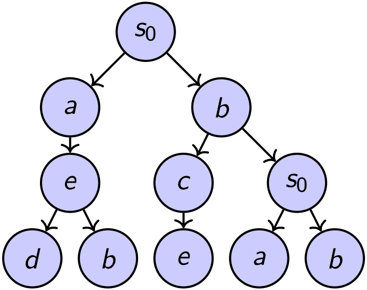

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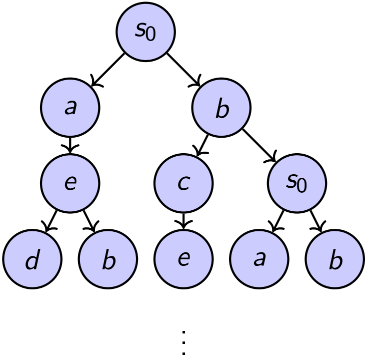

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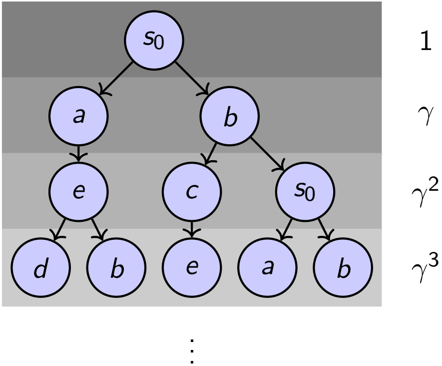

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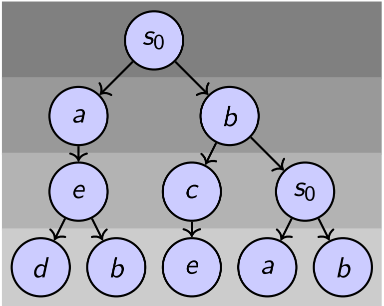

1

γ

γ^2

γ^3

$\vdots$

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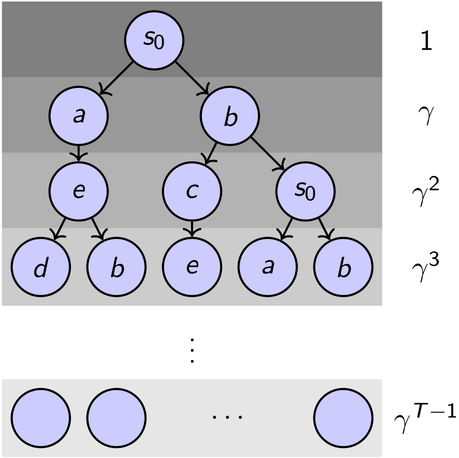

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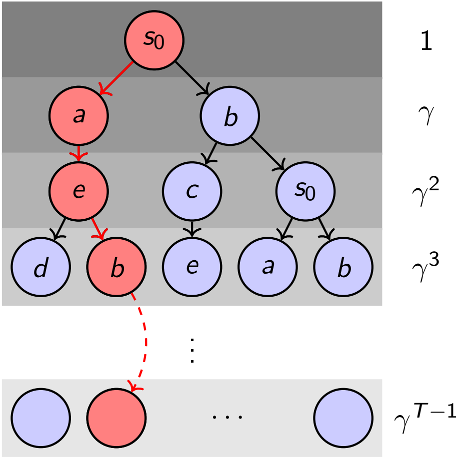

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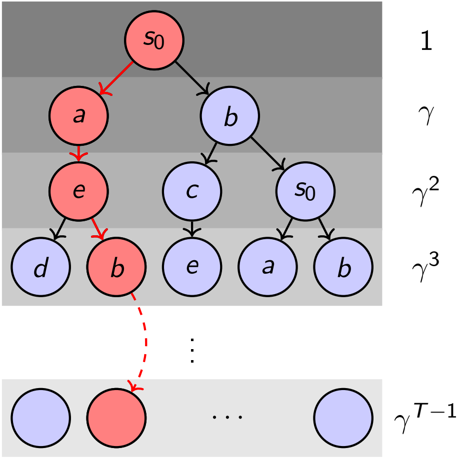

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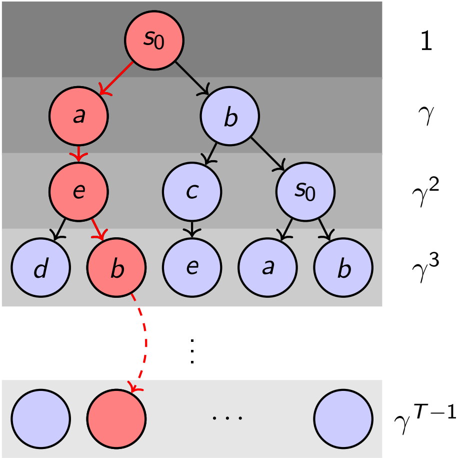
- Value function approximately equal to:

$$V(s_0) = \sum_{\mathbf{s}\in S^{T-1}} \mathbb{P}(\mathbf{s})R(\mathbf{s}) + \mathcal{O}(\varepsilon)$$



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$$|s_0\rangle$$

$$|0\rangle$$

$$|0\rangle$$

$$|0\rangle$$

$$\vdots$$

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$\mathcal{P}$

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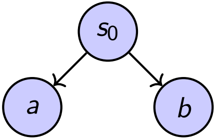

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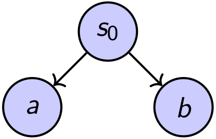

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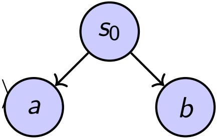

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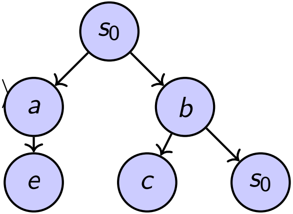

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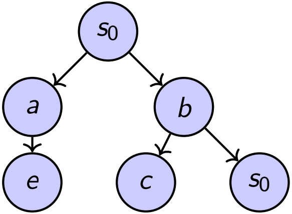

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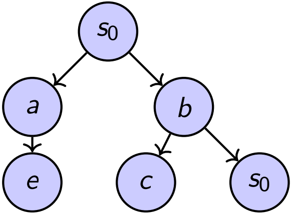
$$\vdots$$

$$|0\rangle$$



QVE step 1: Setting up the tree

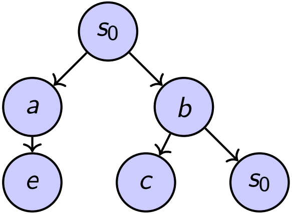
We have access to: $\mathcal{P} : |s\rangle\,|0\rangle \mapsto |s\rangle \sum_{s' \in S} \sqrt{P_{s \to s'}}\,|s'\rangle$

$\mathcal{P}$

$\mathcal{P}$

$\mathcal{P}$

$$\sum_{\mathbf{s} \in S^3} \sqrt{\mathbb{P}(\mathbf{s})}\,|\mathbf{s}\rangle$$



$$\vdots$$

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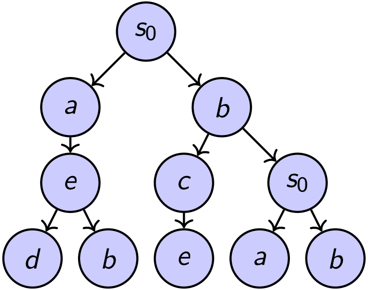
$\mathcal{P}$

$\mathcal{P}$

$$\sum_{\mathbf{s} \in S^3} \sqrt{\mathbb{P}(\mathbf{s})}\,|\mathbf{s}\rangle$$

$\vdots$

$|0\rangle$



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$\mathcal{P}$

$\mathcal{P}$

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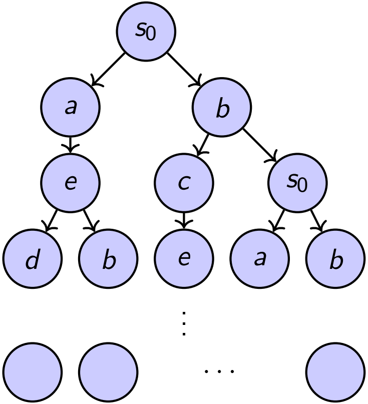
$$\sum_{\mathbf{s} \in S^{T-1}} \sqrt{\mathbb{P}(\mathbf{s})} |\mathbf{s}\rangle$$



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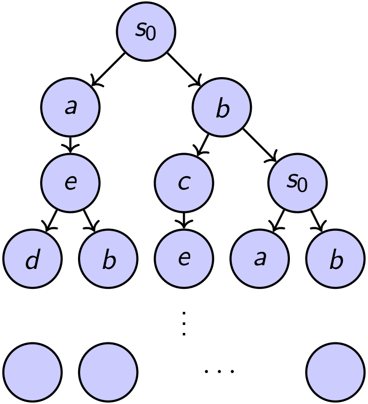

$\overline{\mathcal{P}} : |s_0\rangle |0\rangle^{\otimes(T-1)} \mapsto \sum_{\mathbf{s} \in S^{T-1}} \sqrt{\mathbb{P}(\mathbf{s})} |\mathbf{s}\rangle$ with $T-1$ queries to $\mathcal{P}$

QVE step 2: Calculating the reward for a path

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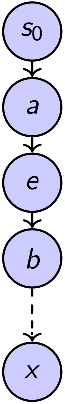

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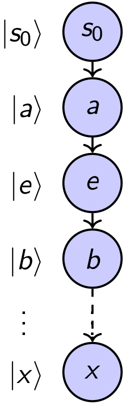

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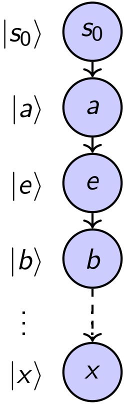

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We have access to:

$$\mathcal{R} : |s\rangle \mapsto e^{iR(s)} |s\rangle$$

Convert:

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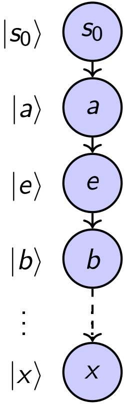

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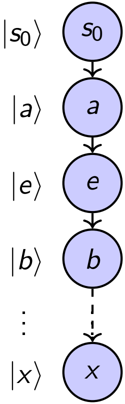
Now multiply by c:

$$|s\rangle |00\rangle \mapsto \sqrt{cR(s)} |s\rangle |11\rangle + |\perp\rangle$$



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Convert back:

$$\mathcal{R}^c : |s\rangle \mapsto e^{icR(s)} |s\rangle$$

$|s_0\rangle$

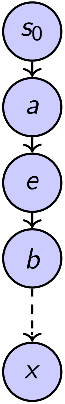
$|a\rangle$

$|e\rangle$

$|b\rangle$

$\vdots$

$|x\rangle$



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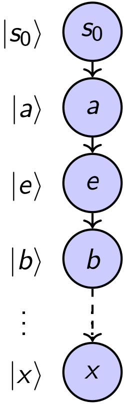
$\mathcal{R}$



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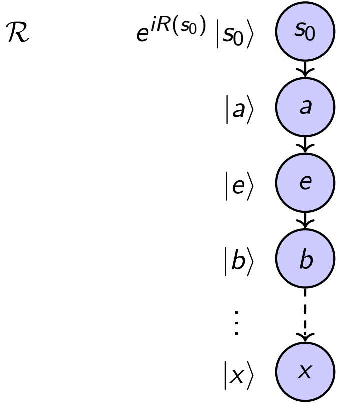

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Convert back:

$$\mathcal{R}^c : |s\rangle \mapsto e^{icR(s)} |s\rangle$$

$\mathcal{R}$ $\quad e^{iR(s_0)} |s_0\rangle$

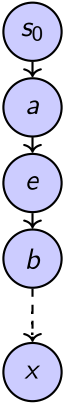
$\mathcal{R}^\gamma$ $\quad |a\rangle$

$|e\rangle$

$|b\rangle$

$\vdots$

$|x\rangle$



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$\mathcal{R}$ $\qquad e^{iR(s_0)} |s_0\rangle$

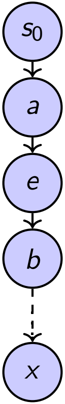
$\mathcal{R}^\gamma$ $\qquad e^{i\gamma R(a)} |a\rangle$

$|e\rangle$

$|b\rangle$

$\vdots$

$|x\rangle$



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$\mathcal{R}$	$e^{iR(s_0)} \|s_0\rangle$	
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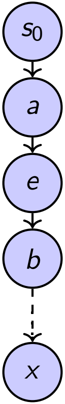
$\mathcal{R}^{\gamma^2}$	$e^{i\gamma^2 R(e)} \|e\rangle$	
	$\|b\rangle$	
	$\vdots$	
	$\|x\rangle$	



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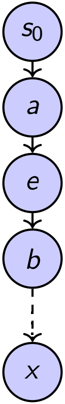
$\mathcal{R}$	$e^{iR(s_0)}\,|s_0\rangle$	s_0
$\mathcal{R}^{\gamma}$	$e^{i\gamma R(a)}\,|a\rangle$	a
$\mathcal{R}^{\gamma^2}$	$e^{i\gamma^2 R(e)}\,|e\rangle$	e
$\mathcal{R}^{\gamma^3}$	$e^{i\gamma^3 R(b)}\,|b\rangle$	b
	$\vdots$	
	$|x\rangle$	x



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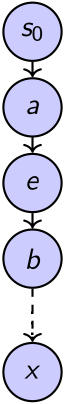
$\mathcal{R}^{\gamma^3}$	$e^{i\gamma^3 R(b)} \|b\rangle$
$\vdots$	$\vdots$
$\mathcal{R}^{\gamma^{T-1}}$	$e^{i\gamma^{T-1} R(x)} \|x\rangle$



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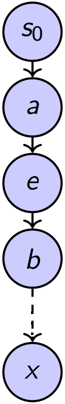

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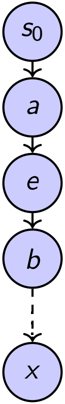

$$|\mathbf{s}\rangle \mapsto e^{iR(\mathbf{s})} |\mathbf{s}\rangle \qquad \text{with } \widetilde{\mathcal{O}}(T) \text{ queries to } \mathcal{R}$$

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$\vdots$ $\quad \vdots$

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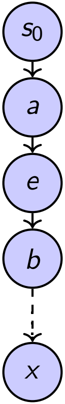

$$|\mathbf{s}\rangle \mapsto e^{iR(\mathbf{s})} |\mathbf{s}\rangle \qquad \text{with } \widetilde{\mathcal{O}}(T) \text{ queries to } \mathcal{R}$$

$$\overline{\mathcal{R}} : |\mathbf{s}\rangle |0\rangle \mapsto \sqrt{R(\mathbf{s})} |\mathbf{s}\rangle |1\rangle + |\perp\rangle \qquad \text{with } \widetilde{\mathcal{O}}(T) \text{ queries to } \mathcal{R}$$

Quantum value estimation algorithm

Quantum value estimation algorithm

- We have constructed the following operations with $\widetilde{\mathcal{O}}(T)$ queries to $\mathcal{P}$ and $\mathcal{R}$:

$$\overline{\mathcal{P}} : |s_0\rangle |0\rangle^{\otimes(T-1)} \mapsto \sum_{\mathbf{s} \in S^{T-1}} \sqrt{\mathbb{P}(\mathbf{s})} |\mathbf{s}\rangle \qquad \text{and} \qquad \overline{\mathcal{R}} : |\mathbf{s}\rangle |0\rangle \mapsto \sqrt{R(\mathbf{s})} |\mathbf{s}\rangle |1\rangle + |\perp\rangle$$

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- We want to calculate:

$$V(s_0) = \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t R(S_t)\right] \approx \sum_{\mathbf{s}\in S^{T-1}} \mathbb{P}(\mathbf{s})R(\mathbf{s})$$

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- Composing $\overline{\mathcal{P}}$ and $\overline{\mathcal{R}}$ yields:

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- Composing $\overline{\mathcal{P}}$ and $\overline{\mathcal{R}}$ yields:

$$|s_0\rangle |0\rangle^{\otimes(T-1)} |0\rangle \overset{\overline{\mathcal{P}}}{\mapsto} \sum_{\mathbf{s} \in S^{T-1}} \sqrt{\mathbb{P}(\mathbf{s})} |\mathbf{s}\rangle |0\rangle \overset{\overline{\mathcal{R}}}{\mapsto} \sum_{\mathbf{s} \in S^{T-1}} \sqrt{\mathbb{P}(\mathbf{s}) R(\mathbf{s})} |\mathbf{s}\rangle |1\rangle + |\perp\rangle$$

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- One can obtain the value function with amplitude estimation up to precision ε with

$$\widetilde{\mathcal{O}}\left(\frac{T|R|_{\max}}{\varepsilon(1-\gamma)}\right) = \widetilde{\mathcal{O}}\left(\frac{|R|_{\max}}{\varepsilon(1-\gamma)^2}\right)$$

queries to $\mathcal{P}$ and $\mathcal{R}$, quadratically faster than classical algorithms.

Quantum value estimation algorithm

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$$V(s_0) = \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t R(S_t)\right] \approx \sum_{\mathbf{s}\in S^{T-1}} \mathbb{P}(\mathbf{s})R(\mathbf{s})$$

- Composing $\overline{\mathcal{P}}$ and $\overline{\mathcal{R}}$ yields:

$$|s_0\rangle\,|0\rangle^{\otimes(T-1)}\,|0\rangle \overset{\overline{\mathcal{P}}}{\mapsto} \sum_{\mathbf{s}\in S^{T-1}} \sqrt{\mathbb{P}(\mathbf{s})}\,|\mathbf{s}\rangle\,|0\rangle \overset{\overline{\mathcal{R}}}{\mapsto} \sum_{\mathbf{s}\in S^{T-1}} \sqrt{\mathbb{P}(\mathbf{s})R(\mathbf{s})}\,|\mathbf{s}\rangle\,|1\rangle + |\perp\rangle$$

- One can obtain the value function with amplitude estimation up to precision ε with

$$\widetilde{\mathcal{O}}\left(\frac{T|R|_{\max}}{\varepsilon(1-\gamma)}\right) = \widetilde{\mathcal{O}}\left(\frac{|R|_{\max}}{\varepsilon(1-\gamma)^2}\right)$$

  queries to $\mathcal{P}$ and $\mathcal{R}$, quadratically faster than classical algorithms.
- This is essentially optimal for $\varepsilon \downarrow 0$, $|R|_{\max} \to \infty$, $\gamma \uparrow 1$.

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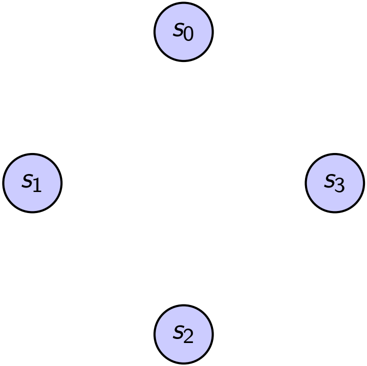

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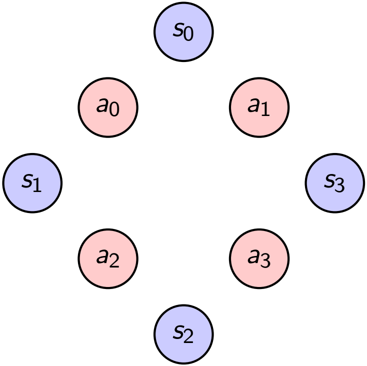

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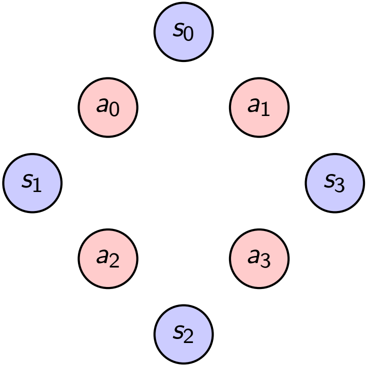

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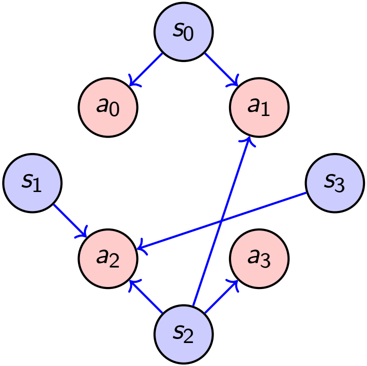

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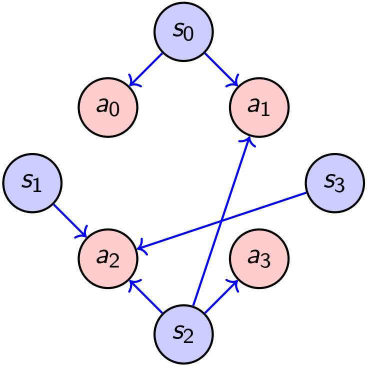

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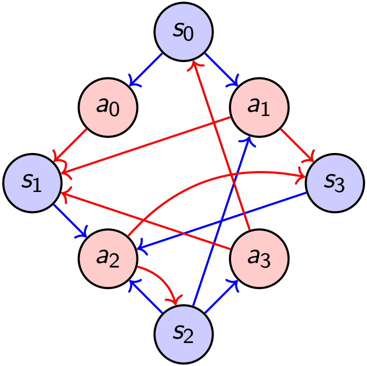

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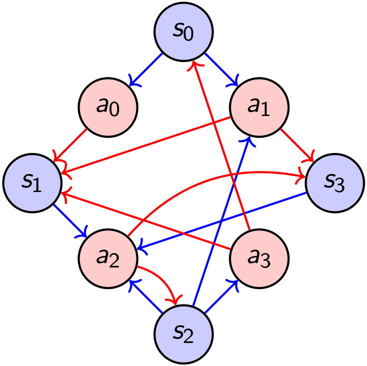

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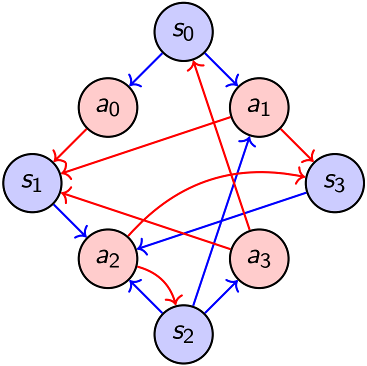

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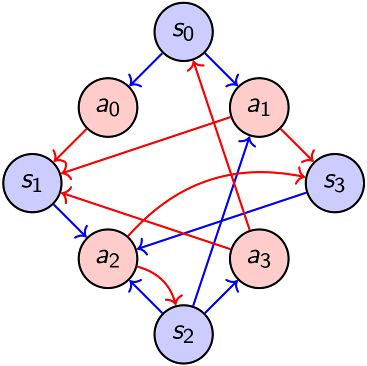

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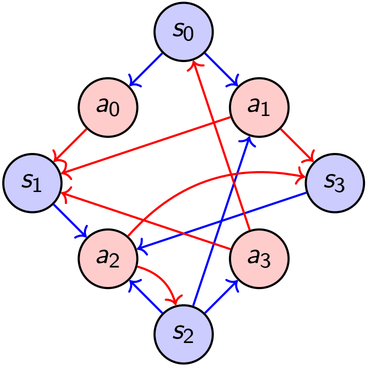

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- How well does it work?

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- Even classical gradient ascent with quantum value evaluation as subroutine provides speed-up!

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Thanks for your attention!

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