Quantum-Inspired Score-Based Variational Inference

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Yuchen's Homepage

Goal: Efficiently approximate complex high-dimensional probability distributions using target score information.

Non-Gaussian variational family
Flexible distribution beyond a single Gaussian shape

Score-based learning
Uses target log-density gradients; no target normalizing constant needed

EigenVI (Cai et al., Neurips 2024)

$$q_\theta(x_1, x_2, \dots, x_D) = \left| \left\langle \theta, \bigotimes_{d=1}^{D} \phi(x_d) \right\rangle \right|^2$$

reformulate → eigenvalue problem

$$\min_\theta \theta^{\mathrm{T}} M \theta, \quad s.t. ||\theta||_F^2 = 1$$

variational model

$$D_F(q_\theta(x) || p(x)) = \int q_\theta(x) \left\| \nabla_x \log p(x) - \nabla_x \log q_\theta(x) \right\|_F^2 dx$$

target distribution — score of target distribution

Limitation of EigenVI

Curse of dimensionality
- The dimension of θ grows exponentially.
- The number of score queries used for estimating M

Degeneracy
- The minimum eigenvalue of M may have multiplicity greater than one, whereas EigenVI uses a single eigenvector.

Ours: QuanVI

Parameterizing ρ with Quantum Tensor Networks (QTNs)

Density Operator

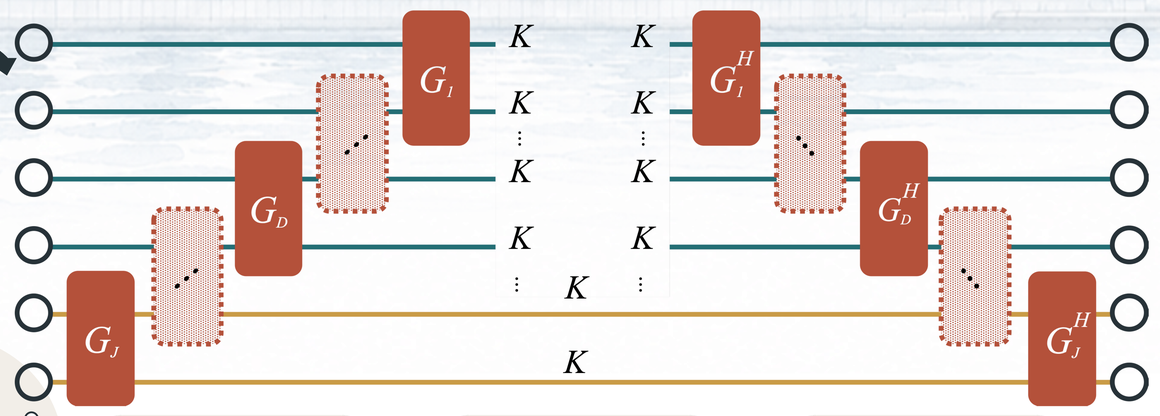
$$\min_\rho tr(\rho M), s.t. \rho \succeq 0, \quad tr(\rho) = 1, \quad rank(\rho) \le r$$

$r = 1$: $\min_\theta \theta^{\mathrm{T}} M \theta, \quad s.t. ||\theta||_F^2 = 1$

general r $(1 \le r \le K^D)$: $\rho \in \mathbb{R}^{K^D \times K^D}$ positive semidefinite (PSD) matrix

$D_F(q_{\rho^*} \| p) \le \mathrm{tr}(\rho^* M)$ reasonable surrogate

Li et al. "On the approximation complexity of matrix product operator (MPO) born machines." arXiv preprint arXiv:2605.11471 (2026).



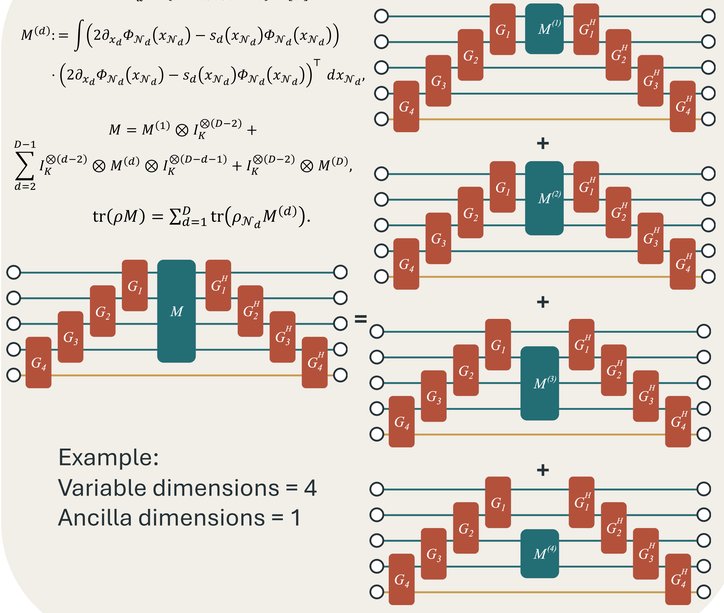
Markov Dependency Assumption

We assume a nearest-neighbor dependency structure, where $s_d(x)$ depends only on the variables in $\mathcal{N}_d := \{d-1, d, d+1\} \cap [D]$.

$$M^{(d)} := \int \left(2\partial_{x_d} \Phi_{\mathcal{N}_d}(x_{\mathcal{N}_d}) - s_d(x_{\mathcal{N}_d}) \Phi_{\mathcal{N}_d}(x_{\mathcal{N}_d})\right) \cdot \left(2\partial_{x_d} \Phi_{\mathcal{N}_d}(x_{\mathcal{N}_d}) - s_d(x_{\mathcal{N}_d}) \Phi_{\mathcal{N}_d}(x_{\mathcal{N}_d})\right)^{\mathrm{T}} dx_{\mathcal{N}_d},$$

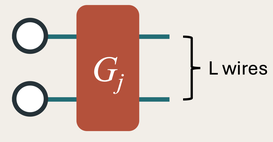
$$M = M^{(1)} \otimes I_K^{\otimes(D-2)} + \sum_{d=2}^{D-1} I_K^{\otimes(d-2)} \otimes M^{(d)} \otimes I_K^{\otimes(D-d-1)} + I_K^{\otimes(D-2)} \otimes M^{(D)},$$

$$\mathrm{tr}(\rho M) = \textstyle\sum_{d=1}^{D} \mathrm{tr}\left(\rho_{\mathcal{N}_d} M^{(d)}\right).$$



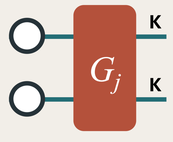
Example:
Variable dimensions = 4
Ancilla dimensions = 1

L Local Window Size



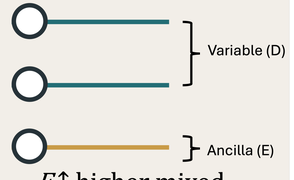
$L\uparrow$ stronger local dependence

K Basis Size



$K\uparrow$ richer representing

E Ancilla Wires



$E\uparrow$ higher mixed states rank

Training

$$\mathcal{L}\left(\{G_j\}_{j=1}^J\right) = \sum_{d=1}^{D} tr\left(\rho_{\mathcal{N}_d} \widetilde{M}^{(d)}\right).$$

Estimate local operators $\widetilde{M}^{(d)}$
↓
Evaluate the loss by QTN contractions
↓
Update gates on the Stiefel manifold

Experiments

Synthetic data result

D	Target	GSM	BAM	ADVI	EigenVI	MoG	QuanVI E0	QuanVI E2
5	Gaussian	0.9520 ±1.3282	$\le 1\times10^{-2}$	$\le 1\times10^{-2}$	$\le 1\times10^{-2}$	0.0152 ±0.0009	$\le 1\times10^{-2}$	$\le 1\times10^{-2}$
	X-shape	2.2494 ±0.4961	3.0904 ±0.2373	1.6816 ±0.0716	0.4007 ±0.0743	1.3039 ±0.0269	**0.2613 ±0.0035**	0.2661 ±0.0054
	GMM3	1.6469 ±0.5895	2.4417 ±0.2273	1.1967 ±0.0313	0.4454 ±0.0613	0.4436 ±0.0617	0.1608 ±0.0112	**0.1598 ±0.0042**
	Funnel	3.3535 ±0.5241	4.8814 ±0.2082	2.8012 ±0.0653	1.3435 ±0.1065	**0.8183 ±0.0742**	4.3944 ±1.8299	2.6412 ±0.4579
	Ring	30.7895 ±8.8223	39.8048 ±2.5664	2.1094 ±0.0221	1.7526 ±0.1454	2.0528 ±0.2233	**0.8861 ±0.0048**	0.8913 ±0.0144
10	Gaussian	$\le 1\times10^{-2}$	$\le 1\times10^{-2}$	$\le 1\times10^{-2}$	OOM	0.0814 ±0.0024	$\le 1\times10^{-2}$	$\le 1\times10^{-2}$
	X-shape	16.0632 ±5.3750	24.9337 ±1.6719	5.8356 ±0.0990	OOM	6.5115 ±0.1666	3.2554 ±0.0670	**3.1928 ±0.0655**
	GMM3	7.0765 ±1.1840	24.0342 ±1.3684	5.4414 ±0.0758	OOM	5.1997 ±0.3525	**3.1225 ±0.0504**	3.1551 ±0.0551
	Funnel	–	29.5528 ±4.4531	7.0246 ±0.0623	OOM	**5.0368 ±0.3313**	9.0460 ±0.8675	8.8288 ±1.0972
	Ring	9.1494 ±1.9204	64.7096 ±1.8813	6.3256 ±0.1146	OOM	7.7603 ±0.4014	3.8400 ±0.0213	**3.8302 ±0.0271**
20	Gaussian	$\le 1\times10^{-2}$	$\le 1\times10^{-2}$	0.0124 ±0.0035	OOM	0.2884 ±0.0088	$\le 1\times10^{-2}$	$\le 1\times10^{-2}$
	X-shape	14.3388 ±2.1860	38.0141 ±2.2533	8.4358 ±0.1412	OOM	9.9434 ±0.2302	**8.1714 ±0.8125**	8.9266 ±0.5087
	GMM3	11.4537 ±0.9701	38.2367 ±0.5113	8.1050 ±0.1880	OOM	8.4863 ±0.4095	**7.4542 ±1.4717**	7.7778 ±1.1659
	Funnel	–	41.6810 ±3.9465	9.8232 ±0.1614	OOM	**7.6320 ±0.2791**	13.1389 ±0.9869	13.4216 ±0.9977
	Ring	13.5824 ±0.2441	77.6129 ±5.2570	**8.9786 ±0.1421**	OOM	10.6938 ±0.3243	9.1621 ±1.5400	9.0459 ±1.0407
100	Gaussian	$\le 1\times10^{-2}$	$\le 1\times10^{-2}$	0.1308 ±0.0020	OOM	2.2290 ±0.0119	$\le 1\times10^{-2}$	$\le 1\times10^{-2}$
	X-shape	75.3810 ±2.1274	186.0990 ±4.2477	47.2649 ±0.2927	OOM	72.7630 ±6.0097	42.2971 ±1.2528	**40.5473 ±4.0462**
	GMM3	73.5309 ±3.1276	187.8098 ±4.1833	47.1609 ±0.2688	OOM	68.3951 ±7.4535	**43.0097 ±2.3348**	43.0798 ±2.9883
	Funnel	85.7464 ±3.1931	188.2434 ±3.0382	48.8944 ±0.2271	OOM	57.0316 ±0.4351	**46.4010 ±3.1020**	47.0005 ±3.8384
	Ring	73.7223 ±2.1166	224.9920 ±4.1197	48.1236 ±0.2075	OOM	76.9241 ±2.1116	43.7935 ±1.0249	**43.1974 ±1.5993**

Real-world data result

Model	D	GSM	BAM	ADVI	MoG	NF	EigenVI	QuanVI $E=0$	QuanVI $E=2$
gpregr	3	1.2107 ±0.0345	1.1962 ±0.0293	1.1509 ±0.0177	7.6146 ±3.9904	3.3739 ±0.4973	**0.0828 ±0.0681**	0.2180 ±0.0463	0.2330 ±0.0369
hmm	4	148.1225 ±2.5882	139.7349 ±3.9980	168.9795 ±32.6976	–	–	**4.0295 ±1.5069**	5.0783 ±0.6214	4.8047 ±0.4491
bball	6	749.1771 ±2.5298	19.9691 ±0.6849	746.7151 ±2.0978	–	–	18.5057 ±3.0322	13.7126 ±0.5198	**13.4460 ±0.3597**

Ablation study on L (local window size)

D	Target	$L=1$	$L=2$	$L=3$	$L=4$	$L=5$
5	X-shape	6.773 ±0.040	0.265 ±0.007	0.248 ±0.005	0.255 ±0.008	0.246 ±0.012
	GMM3	9.266 ±4.613	0.160 ±0.004	0.156 ±0.005	0.155 ±0.007	0.155 ±0.005
	Funnel	9.299 ±2.148	2.838 ±1.262	1.606 ±0.212	1.388 ±0.093	1.481 ±0.265
	Ring	11.050 ±3.082	0.879 ±0.018	0.891 ±0.025	0.919 ±0.027	0.893 ±0.024
10	X-shape	16.203 ±1.615	3.212 ±0.069	2.956 ±0.053	2.859 ±0.053	2.869 ±0.060
	GMM3	19.865 ±5.100	3.146 ±0.065	2.905 ±0.049	2.734 ±0.068	2.728 ±0.097
	Funnel	18.983 ±3.115	7.929 ±1.195	6.367 ±0.435	4.383 ±0.527	2.812 ±0.050
	Ring	20.669 ±3.089	3.822 ±0.047	3.580 ±0.074	3.450 ±0.060	3.343 ±0.064
20	X-shape	36.863 ±2.211	7.914 ±1.599	7.709 ±0.350	7.636 ±0.290	–
	GMM3	35.936 ±2.577	8.331 ±0.415	7.740 ±0.141	7.543 ±0.137	–
	Funnel	38.551 ±5.300	13.766 ±0.583	11.773 ±0.185	7.007 ±0.234	–
	Ring	42.651 ±4.803	9.159 ±0.646	8.369 ±0.364	7.942 ±0.140	–

Ablation study on K (basis size)

D	Target	$K=1$	$K=2$	$K=3$	$K=4$	$K=5$	$K=6$	$K=7$	$K=8$	$K=9$	$K=10$
5	X-shape	2.024 ±0.010	1.282 ±0.022	0.863 ±0.023	0.433 ±0.007	0.265 ±0.007	0.157 ±0.005	0.072 ±0.004	0.033 ±0.003	0.024 ±0.003	**0.012** ±0.001
	GMM3	2.198 ±0.029	1.338 ±0.015	0.846 ±0.029	0.363 ±0.011	0.160 ±0.004	0.145 ±0.006	0.049 ±0.002	0.029 ±0.004	0.020 ±0.001	**0.008** ±0.000
	Funnel	2.141 ±0.033	2.059 ±0.282	**1.593** ±0.117	3.937 ±1.857	2.838 ±1.262	2.876 ±0.181	3.488 ±0.317	3.927 ±0.074	4.247 ±0.154	4.629 ±0.348
	Ring	4.700 ±0.017	2.441 ±0.028	1.595 ±0.028	1.585 ±0.032	0.879 ±0.018	0.447 ±0.013	0.289 ±0.004	1.025 ±0.025	0.276 ±0.005	**0.108** ±0.004
10	X-shape	4.831 ±0.029	4.453 ±0.024	4.399 ±0.106	3.962 ±0.153	3.212 ±0.069	2.923 ±0.092	1.865 ±0.029	0.948 ±0.036	**0.787** ±0.037	14.654 ±1.949
	GMM3	4.984 ±0.032	4.486 ±0.057	4.486 ±0.053	3.994 ±0.077	3.146 ±0.065	2.957 ±0.039	1.772 ±0.063	1.005 ±0.042	**0.823** ±0.078	13.896 ±0.996
	Funnel	**4.934** ±0.037	5.106 ±0.197	5.220 ±0.134	7.851 ±1.292	7.929 ±1.195	8.453 ±0.844	9.420 ±0.761	8.129 ±1.184	11.118 ±0.511	12.922 ±0.716
	Ring	7.488 ±0.035	5.577 ±0.095	5.144 ±0.029	5.125 ±0.102	3.822 ±0.047	3.241 ±0.131	2.056 ±0.050	1.937 ±0.047	**1.062** ±0.045	15.105 ±1.830
20	X-shape	10.268 ±0.088	6.410 ±0.106	9.515 ±0.209	8.481 ±1.162	7.914 ±1.599	7.996 ±0.677	**5.289** ±1.775	5.751 ±1.048	5.345 ±0.896	25.636 ±4.765
	GMM3	10.407 ±0.039	6.360 ±0.054	10.067 ±0.752	9.254 ±0.486	8.331 ±0.415	8.177 ±1.017	6.399 ±1.763	5.545 ±1.195	4.801 ±1.391	**4.346** ±1.101
	Funnel	10.331 ±0.073	**7.110** ±0.328	10.671 ±0.397	13.264 ±1.533	13.766 ±0.583	14.424 ±0.430	14.322 ±0.513	14.617 ±0.698	15.645 ±1.036	20.068 ±0.902
	Ring	12.870 ±0.052	7.555 ±0.074	10.416 ±0.190	10.280 ±0.426	9.159 ±0.646	8.074 ±0.895	**5.483** ±1.505	5.603 ±1.437	5.543 ±1.176	21.898 ±0.972

Ablation study on E (Ancilla wires)

D	Target	$E=0$	$E=1$	$E=2$	$E=3$	$E=4$	$E=5$	$E=6$	$E=7$	$E=8$	$E=9$	$E=10$
5	X-shape	0.436 ±0.162	0.350 ±0.050	0.388 ±0.040	0.392 ±0.052	0.396 ±0.038	**0.349** ±0.016	–	–	–	–	–
	GMM3	**0.173** ±0.023	0.195 ±0.021	0.202 ±0.033	0.206 ±0.031	0.203 ±0.014	0.214 ±0.075	–	–	–	–	–
	Funnel	3.131 ±0.553	2.985 ±0.562	3.763 ±0.782	3.434 ±0.811	3.193 ±0.342	**2.670** ±0.714	–	–	–	–	–
	Ring	1.054 ±0.143	0.967 ±0.066	1.063 ±0.204	1.083 ±0.180	**0.927** ±0.035	1.046 ±0.123	–	–	–	–	–
10	X-shape	**3.211** ±0.224	3.382 ±0.142	3.253 ±0.188	3.334 ±0.135	3.339 ±0.250	3.415 ±0.195	3.277 ±0.241	3.321 ±0.100	3.385 ±0.177	3.470 ±0.198	3.366 ±0.244
	GMM3	3.405 ±0.343	3.283 ±0.269	3.216 ±0.099	3.309 ±0.104	3.250 ±0.125	3.206 ±0.255	3.340 ±0.324	3.239 ±0.184	**3.091** ±0.166	3.244 ±0.206	3.234 ±0.136
	Funnel	9.052 ±1.045	8.781 ±0.682	8.772 ±0.581	9.151 ±0.397	8.603 ±0.808	8.688 ±1.054	9.063 ±0.322	8.614 ±0.840	9.084 ±0.486	8.680 ±0.808	**7.870** ±0.844
	Ring	3.948 ±0.187	4.086 ±0.398	3.956 ±0.308	3.912 ±0.284	**3.829** ±0.191	3.958 ±0.117	3.966 ±0.099	4.073 ±0.254	3.953 ±0.249	4.063 ±0.122	4.052 ±0.126
20	X-shape	8.294 ±1.607	7.664 ±1.668	7.947 ±1.502	8.764 ±1.985	8.093 ±0.189	**6.971** ±1.486	8.519 ±0.607	8.062 ±1.324	7.306 ±1.071	8.374 ±1.411	8.491 ±1.104
	GMM3	8.021 ±0.862	7.944 ±1.242	7.916 ±1.518	8.068 ±0.772	8.552 ±0.452	8.500 ±1.484	8.646 ±0.715	8.308 ±0.442	**7.648** ±1.396	8.213 ±0.556	8.154 ±1.810
	Funnel	13.143 ±1.655	13.480 ±0.675	12.637 ±1.569	13.677 ±0.840	13.661 ±0.550	12.756 ±1.658	13.536 ±1.518	13.543 ±0.657	**12.345** ±1.369	13.405 ±1.369	12.843 ±1.085
	Ring	8.080 ±1.067	7.945 ±1.077	8.285 ±1.318	8.726 ±1.454	7.829 ±1.846	8.691 ±1.005	7.532 ±1.904	9.348 ±0.442	8.062 ±1.856	9.374 ±0.495	**7.407** ±1.978

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