

Local and Multi-Scale Strategies to Mitigate Exponential Concentration in Quantum Kernels (#6)

Checkpoint 2

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1 Project overview

Quantum kernels embed classical inputs into quantum states and use **state overlap** as a similarity score for kernel methods (e.g., SVMs). A key limitation is **exponential concentration**: as qubit count and/or circuit depth grows, kernel matrices drift toward the identity (off-diagonals near zero), reducing separability.

We implement and benchmark two mitigation strategies:

- **Local (patch-wise) kernels:** compute similarity on **subsystems** (patches) via reduced density matrices (RDMs), then aggregate across patches.
- **Multi-Scale kernels:** compute kernels at multiple granularities (local + global) and combine them via a **non-negative weighted mix**.

2 Progress made

We built a reproducible, end-to-end benchmarking pipeline:

- Baseline / local / multi-scale kernels under a shared API.
- TOML-driven runner (`scripts/run_experiment.py`) + multi-config orchestrator (`scripts/run_all_benchmarks.py`).
- Diagnostics + evaluation: off-diagonal histograms, eigen-spectra, and SVM with precomputed kernels.
- Stable run IDs and cross-platform path handling for reliable aggregation.

3 Explorations and experiments

We validated the pipeline on toy datasets (`make_circles`, `iris`) and focused the main concentration study on real datasets: `breast_cancer` and `parkinsons`, sweeping **dimension d (qubits/features)** while keeping comparisons matched (same feature map, depth, entanglement, backend, centered, normalization and split policy).

4 Key insights and learnings

4.1 Matched comparisons (uncentered, d=8 examples)

4.1.1 `breast_cancer` (n=569, d=8): `zz_manual_canonical`, `depth=1`, `ent=ring`, `centered=False`

Kernel	Scales / Patches	Weights	OffDiag $\mu \pm \sigma$	EffRank	Align	Val	Test
baseline	all qubits	-	0.012 ± 0.030	475.8	0.073	0.781	0.675
local	$2q \times 4$	-	0.312 ± 0.091	75.0	0.090	0.754	0.728
multiscale	$2q \times 4 + 8q \times 1$	[0.5, 0.5]	0.193 ± 0.060	184.7	0.094	0.807	0.719

Table 1: Breast cancer (8 qubits): baseline vs local vs multi-scale (matched, uncentered).

Reading: baseline shows the strongest concentration signature (off-diags ~ 0); local is best on test (0.728), multi-scale is competitive.

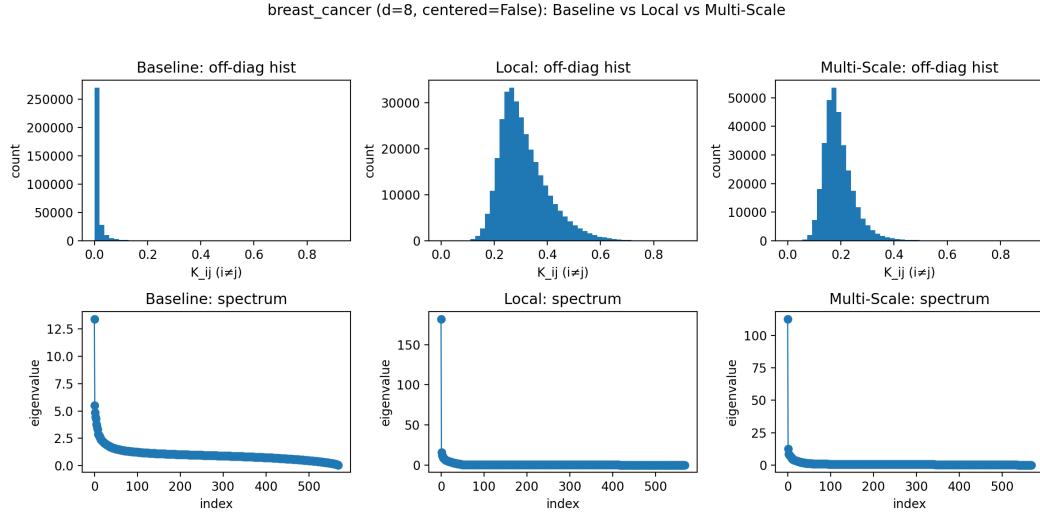


Figure 1: Breast Cancer (8 qubits): local and multi-scale shift off-diagonals away from 0 and reshape the spectrum relative to baseline.

4.1.2 `parkinsons` (n=195, d=8): `zz_qiskit`, `depth=1`, `ent=linear`, `centered=False`

Kernel	Scales / Patches	Weights	OffDiag $\mu \pm \sigma$	EffRank	Align	Val	Test
baseline	all qubits	-	0.004 ± 0.008	193.6	0.072	0.769	0.795
local	$2q \times 4$	-	0.250 ± 0.064	63.2	0.046	0.769	0.795
multiscale	$2q \times 4 + 8q \times 1$	[0.5, 0.5]	0.154 ± 0.042	113.6	0.060	0.769	0.795

Table 2: Parkinsons (8 qubits): baseline vs local vs multi-scale (matched, uncentered).

Reading: local reduces concentration strongly, but learning metrics do not improve in this sweep; this points to patch/feature-map/depth retuning.

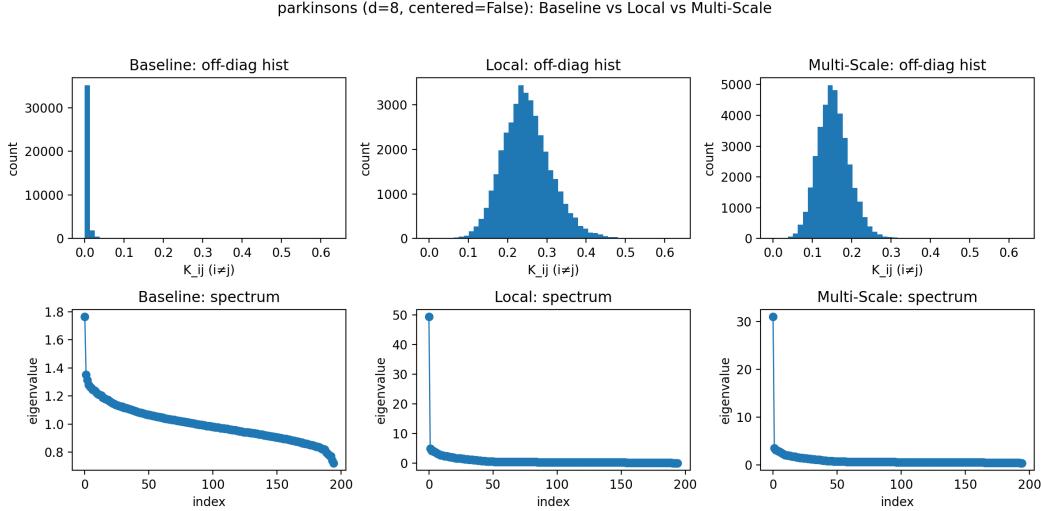


Figure 2: Parkinsons (8 qubits): local/multi-scale reduce concentration vs baseline, but no SVM gain here.

4.2 Scaling with dimension

To directly test that concentration happens when we increase the dimension, we ran $d = 4, 6, 8, 10, 12, 14, 16, 18, 20$ for both `breast_cancer` and `parkinsons` (matched settings, uncentered kernels).

What we observe (both datasets):

- **Baseline concentrates rapidly with d :** off-diagonal median (p50) and tail (p95) drop toward ~ 0 , consistent with “kernel \rightarrow identity”.
- **Local and multi-scale mitigate concentration across all d :** p50/p95 stay far from 0, and the kernel spectrum stays structured.
- **Multi-scale is intentionally intermediate:** because it mixes global+local, it typically lands between baseline and pure-local in concentration metrics.

Performance link (so far):

- On `breast_cancer`, local/multi-scale remain competitive vs baseline across d (local often best).
- On `parkinsons`, concentration is reduced but **test accuracy is largely flat** across d , suggesting that “less concentration” alone is not sufficient without better patch design / feature-map / depth.

4.3 Plots vs d

Breast cancer (d sweep): include at least p50 + effective-rank (also p95 + test acc). See Figures 3, 4, 5, 6.

Parkinsons (d sweep): same structure. See Figures 7, 8, 9, 10.

5 Technical challenges

- Cross-platform reproducibility: path/cwd issues fixed by resolving configs/outputs relative to repo root.
- Reliable aggregation at scale: stable run IDs + path normalization for robust joins.
- Numerical stability: consistent symmetrization, optional small diagonal regularization.

6 Current status

- End-to-end pipeline runs baseline/local/multi-scale and produces diagnostics + summaries.
- **Main result so far:** baseline concentration worsens sharply as d increases, while local/multi-scale maintain non-trivial kernel structure across d ; performance gains are dataset-dependent.

7 Path forward

1. Improve patch design (overlapping / structured patches; try 1q/2q/3q mixes).
2. Weight selection: choose multi-scale weights via validation, then report test once.
3. Probe depth sensitivity (depth>1) once patch design is stable.
4. Add lightweight robustness checks (input noise / sampling noise).

MVP target: show at least one dataset where local or multi-scale yields a clear advantage (accuracy and/or robustness), supported by reduced concentration and improved kernel structure.

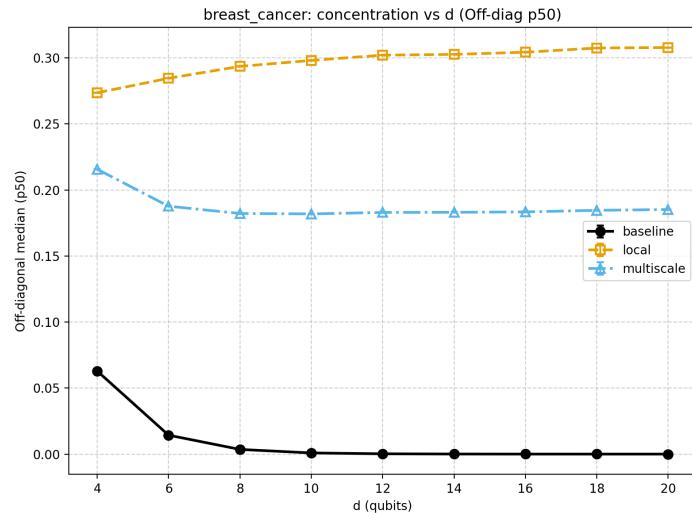


Figure 3: breast_cancer: concentration vs d (Off-diag p50).

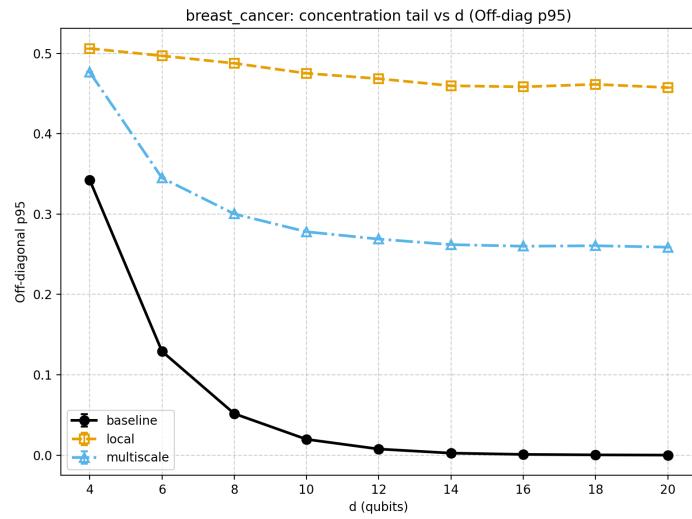


Figure 4: breast_cancer: concentration tail vs d (Off-diag p95).

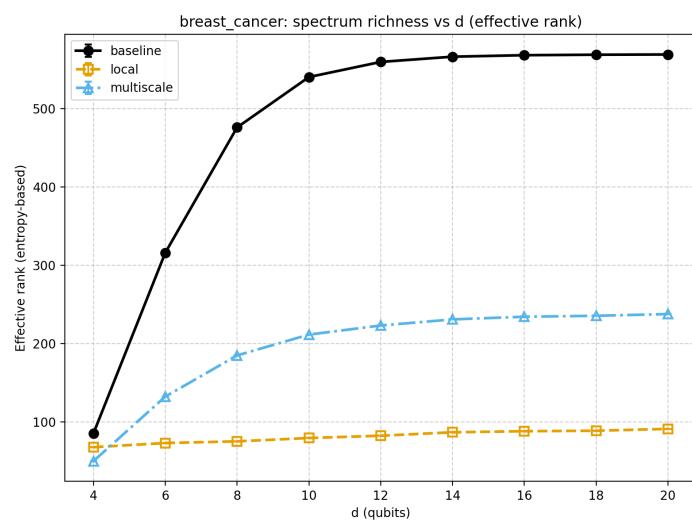


Figure 5: breast_cancer: spectrum richness vs d (effective rank).

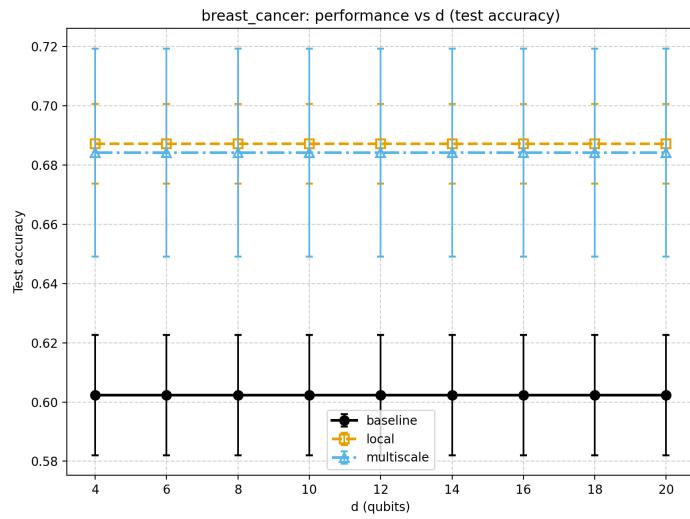


Figure 6: breast_cancer: performance vs d (test accuracy).

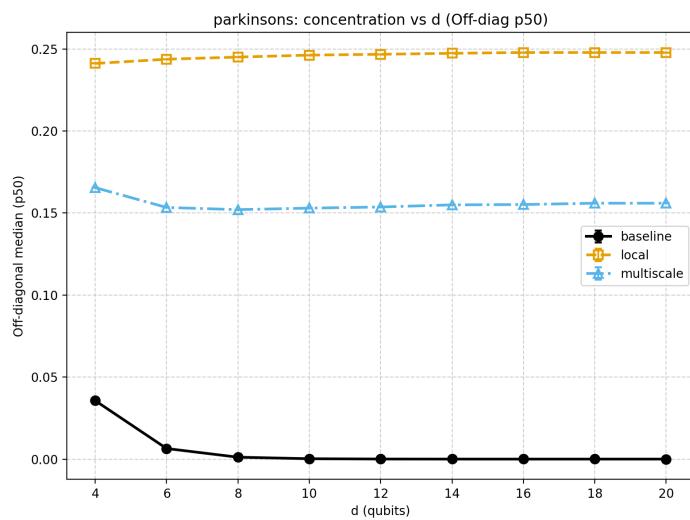


Figure 7: parkinsons: concentration vs d (Off-diag p50).

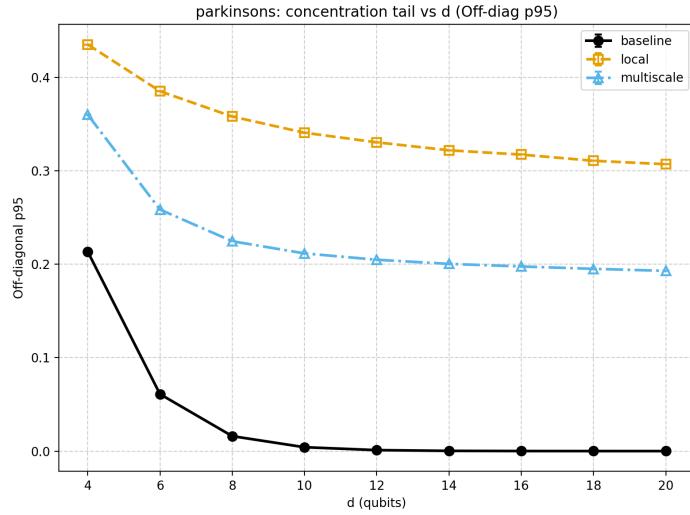


Figure 8: parkinsons: concentration tail vs d (Off-diag p95).

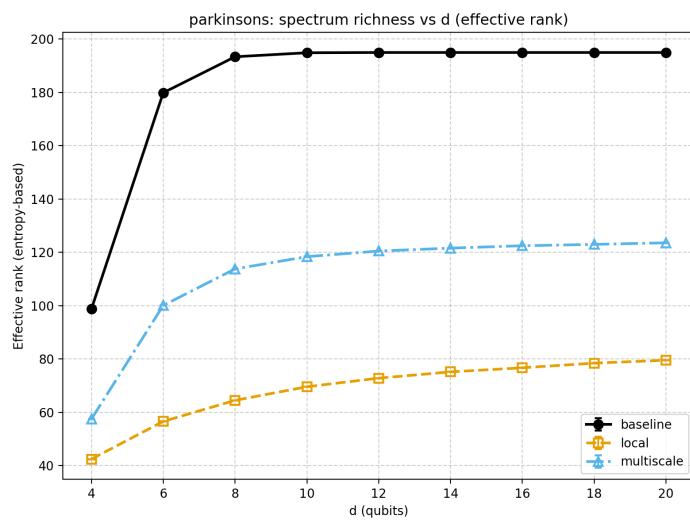


Figure 9: parkinsons: spectrum richness vs d (effective rank).

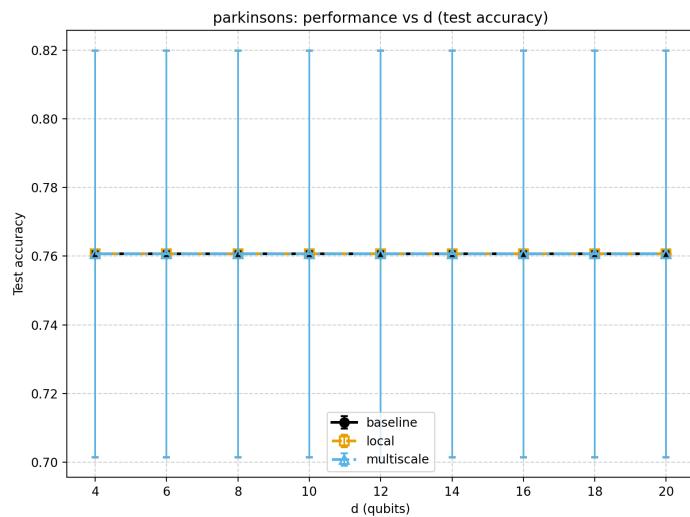


Figure 10: parkinsons: performance vs d (test accuracy).