

GRAMA: Quantum Kernels for Multi-Omics

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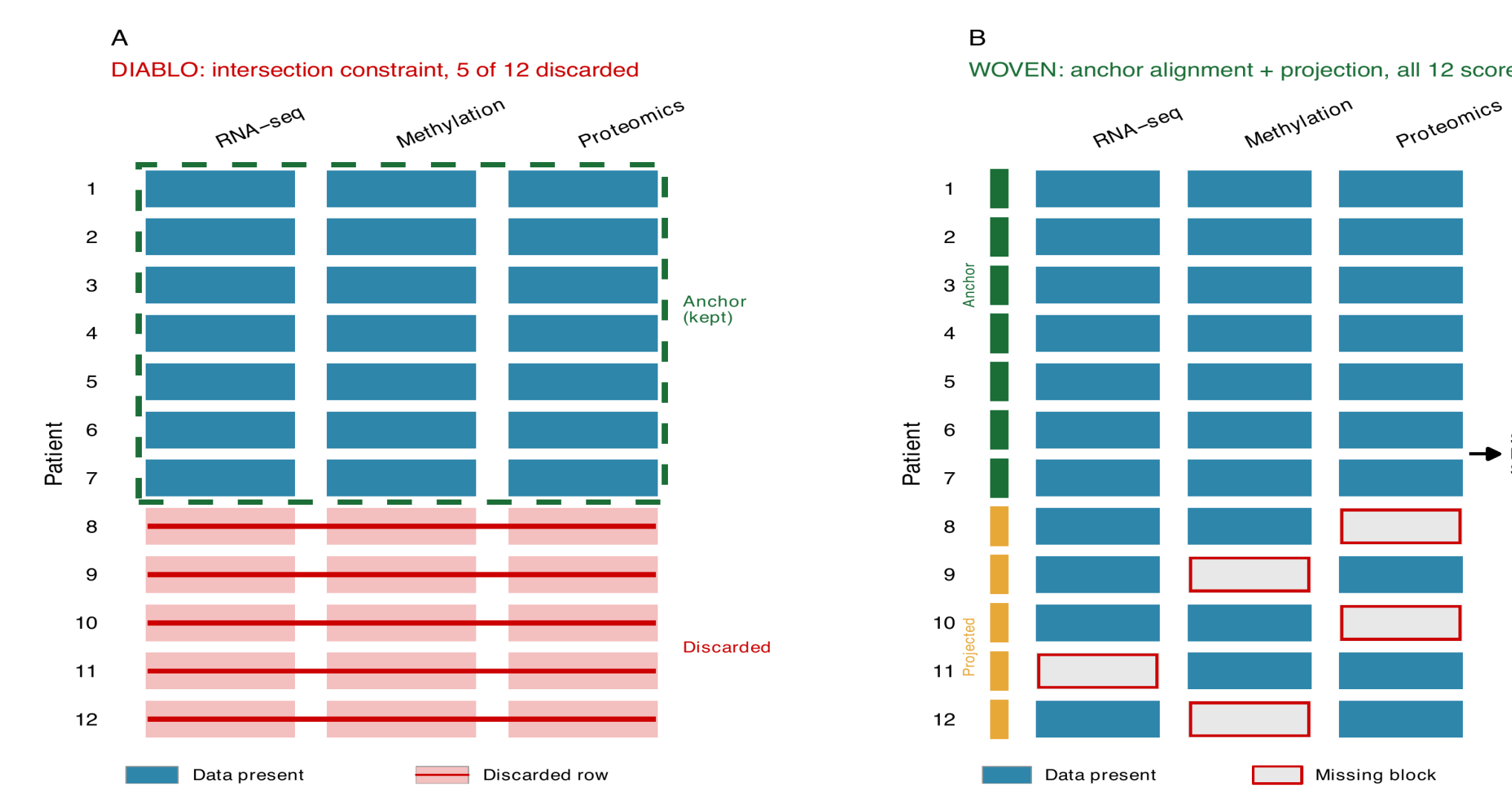


Motivation

- Multi-omics integration combines transcriptomic, epigenomic, proteomic, metabolomic, and microbiome data to characterize disease.
- Real cohorts are “ragged”: patients routinely miss entire data modalities from failed assays or missed visits.
- The field standard (DIABLO) deletes any patient missing even one modality, discarding power and disproportionately excluding the sickest patients.
- Question: can a quantum kernel encoding cross-feature interactions improve multi-view alignment under missingness, without discarding incomplete patients?

Methods

- GRAMA aligns modalities in a shared latent space using only fully-observed “anchor” patients (supervised dual multi-view CCA, single closed-form eigendecomposition).
- A graph Laplacian, built from all available patients, regularizes toward local structure; incomplete patients are projected directly from observed views, no imputation.
- Quantum extension: the classical RBF kernel is replaced by a ZZ-Feature Map fidelity kernel (Qiskit), the only step that differs between GRAMA-RBF and GRAMA-Quantum.



Ablation



Key Results

- Effective sample size: GRAMA retains 100% of patients at every missingness level; DIABLO retains only 48% (30% missing) and 27% (50% missing).
- Complete data: GRAMA-Quantum gives the best cluster geometry and label recovery of the three methods (silhouette 0.376, NMI 0.684).
- 50% missing: GRAMA-Quantum modestly outperforms GRAMA-RBF (BER 0.491 vs. 0.499; NMI 0.188 vs. 0.170), consistent with its theoretical edge on the nonlinear class boundary.
- DIABLO's apparently lower BER under missingness is a cherry-picking artifact: it only ever scores its easiest, fully-observed subset of patients.

QPU Validation

- Confirmatory run on real IBM hardware (ibm_kingston, Eagle processor): 30 subjects, 4 qubits (PCA-reduced), 512 shots/circuit, completed in 3m41s of a 5-minute budget.
- Resulting Gram matrices were symmetric and positive semi-definite (min eigenvalue > 0.28), with diagonal means (0.939, 0.946) matching the expected shot-noise floor plus real device noise.
- Confirms the quantum kernel is a valid, physically realizable kernel, not only a simulator result.
- QPU job IDs: d8td9odposuc738oi7ug, d8tdaj5bh0os73epeq7g.

Next Steps

Classical backbone released as an open-source R package (WOVEN), in Bioconductor review; validated on 2,422 real ADNI patients (70% scored vs. 31% for DIABLO).

Demonstrates a clean, isolated quantum-kernel use case in multi-omics biology.

Next: larger-scale ablation for statistical significance; quantum-extension workshop paper.

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Havlicek et al. 2019, Nature; Singh et al. 2019, Bioinformatics (DIABLO).