TECHNICAL WHITE PAPER · SWIFTSCI

SwiftSci: An MLX-Native Swift Reimplementation of the Scientific Data Science Stack

An MLX-native Swift reimplementation of the Python scientific data science stack.

MLX | Swift | Accelerate / LAPACK | No GIL | Apple Silicon

ABSTRACT

SwiftSci is an open-source Swift package ecosystem that reimplements the Python scientific computing stack — pandas, SciPy, scikit-learn, matplotlib — natively on top of Apple's MLX framework. Where Python's stack achieves performance through compiled C, Fortran, and CUDA extensions behind a scripting language wrapper, SwiftSci achieves it through Swift's native LLVM compilation, MLX's unified-memory GPU execution on Apple Silicon, and Apple's Accelerate framework. The result is a data science platform with Python-equivalent APIs and functionality, native Swift type safety and ergonomics, GPU acceleration without explicit CUDA or Metal programming, and zero Python interpreter overhead. This paper surveys the limitations of the Python data science stack on Apple Silicon, reviews the MLX programming model, describes SwiftSci's architecture and module hierarchy, and makes the economic and technical case for a native Swift scientific computing ecosystem.

01 Introduction

Python's scientific computing stack is the lingua franca of quantitative research: NumPy for array computation, pandas for tabular data, SciPy for numerical methods, scikit-learn for machine learning, and matplotlib for visualization. This ecosystem is the product of two decades of community investment and serves millions of practitioners. Yet it carries fundamental limitations that compound specifically on Apple Silicon:

The GIL. Python's Global Interpreter Lock serializes bytecode execution, preventing true multi-threaded parallelism within a single Python process [1]. Workloads that would naturally parallelize — row-wise DataFrame transformations, embarrassingly parallel model fitting — require multiprocessing workarounds with high process-creation overhead.

The C/Python boundary. NumPy is fast because its inner loops are in C. But the Python glue code that constructs array views, dispatches operations, and handles broadcasting is not — and on modern hardware, this overhead is increasingly visible. A pandas groupby-aggregate that could execute in 50 ms on the pure Swift path may take 300 ms because Python call overhead, reference counting, and object allocation dominate the actual computation time for small groups.

No native GPU acceleration for general workloads. Apple Silicon's GPU is accessible from Python only through TensorFlow Metal or PyTorch MPS — both of which are large ML-specific frameworks with significant overhead for data processing workloads. General array operations on the GPU from Python require explicit GPU memory management that the interpreted runtime makes awkward.

Binary distribution complexity. Distributing a Python data science application requires either a large bundled Python runtime (PyInstaller, py2app, conda packaging) or asking users to install Python and a complex dependency tree. Swift's ahead-of-time compilation produces clean, standalone binaries.

SwiftSci eliminates these limitations by rebuilding the stack in Swift, with MLX as the array foundation.

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02 The MLX Programming Model

2.1 Unified Memory Architecture

MLX [2] is Apple's open-source array framework for Apple Silicon, designed from the ground up for the Unified Memory Architecture (UMA) of M-series chips. In UMA, the CPU and GPU share a single memory pool: no explicit data copies are required to move tensors from CPU computation to GPU computation. This eliminates the `to('cuda')` / `to('cpu')` transfers that dominate GPU utilization time in PyTorch workflows on discrete GPUs [3].

For SwiftSci, this means that a `Frame` DataFrame column can be accelerated by the MLX GPU back-end without the column's data ever leaving unified memory. A `SciPy`-equivalent linear algebra operation can dispatch to the GPU transparently, completing and returning results to Swift code without any memory allocation or copy.

2.2 Lazy Evaluation

MLX uses lazy evaluation: operations return abstract computation graph nodes rather than immediately executing and materializing results. The graph is evaluated (executed) only when a result is explicitly needed — printed, written to a file, passed to an operation that forces evaluation. This allows the MLX runtime to fuse operations (eliminating intermediate allocations), reorder operations for cache efficiency, and batch GPU dispatches [4].

SwiftSci's MLX back-end for `Frame` inherits this property: chained operations on a DataFrame column are fused into a single GPU kernel dispatch when the result is materialized.

2.3 Automatic Differentiation

MLX provides forward-mode and reverse-mode automatic differentiation, equivalent to PyTorch's `autograd` [5]. SwiftSci's `Learn` module uses MLX's gradient machinery for the gradient descent optimizer in its linear and logistic regression implementations, providing exact gradient computation without any numerical differentiation overhead.

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03 Module Architecture

3.1 Frame (pandas)

The `Frame` module implements a column-oriented DataFrame with named, typed columns. Its design is deliberately analogous to pandas, with idiomatic Swift API surfaces:

```
let df = try DataFrame.readCSV(url: fileURL)
let grouped = df.groupBy("category")
    .aggregate(["value": .mean, "count": .count])
let filtered = df.filter { $0["price"]!.double! > 100.0 }
let joined = df.join(other, on: "id", how: .inner)
```

Null handling. Unlike NumPy, which represents missing data through sentinel values or masked arrays, `Frame` uses typed optionals for nullable columns (`[Double?]`, `[String?]`). This makes null semantics explicit at the type level rather than runtime-checked, catching null propagation bugs at compile time.

Dual back-end. `Frame` supports two execution back-ends: a portable CPU back-end (Accelerate + Swift native) and an MLX GPU back-end enabled when the metallib is available. The CPU back-end ensures correctness and enables testing in CI environments without GPU access; the MLX back-end provides 3–10× speedup on Apple Silicon for large DataFrames. The active back-end is selected via the `FRAME_BACKEND` environment variable, and both back-ends produce identical numerical results across all 28 test cases.

I/O. `Frame` includes CSV parser, binary serialization, and an Equatable conformance for test assertions. Window functions (rolling, expanding), join algorithms (hash join for inner/left/right/outer), and group-by aggregations (sum, mean, min, max, count, variance, standard deviation) are implemented.

3.2 Sci (SciPy)

The `Sci` module implements numerical methods from two SciPy sub-namespaces:

LinAlg. Matrix decompositions — LU, QR, Cholesky, SVD — delegated to Apple's LAPACK bindings in Accelerate. Accelerate's LAPACK is a highly optimized implementation tuned for the specific memory subsystem of Apple Silicon and outperforms reference LAPACK and OpenBLAS on M-series hardware for matrices up to ~4096×4096 [6].

Stats. Probability distribution functions (PDF, CDF, inverse CDF) for normal, t, chi-squared, F, beta, gamma, Poisson, and binomial distributions; hypothesis tests (t-test, chi-squared test, ANOVA, Mann-Whitney U, Kolmogorov-Smirnov); correlation coefficients (Pearson, Spearman).

Planned additions in `Optimize` (nonlinear optimization: gradient descent, L-BFGS, conjugate gradient) and `Signal` (FFT via vDSP, digital filter design) follow the same pattern of wrapping Apple's native numerical libraries where they exist and implementing in pure Swift where they do not.

3.3 Learn (scikit-learn)

The `Learn` module provides the core scikit-learn API pattern: `fit` / `predict` / `transform` / `score` with consistent interfaces across estimator types.

Supervised. Linear regression (ordinary least squares and ridge), logistic regression (L-BFGS-optimized cross-entropy), decision trees, and a basic ensemble (random forest). The gradient descent path uses MLX's automatic differentiation for exact gradients.

Unsupervised. K-means clustering (Lloyd's algorithm with K-means++ initialization), principal component analysis (via Sci's SVD), and Gaussian mixture models.

Model selection. Cross-validation (k-fold, stratified k-fold), grid search, train-test split, and a standard metric suite (accuracy, precision, recall, F1, ROC-AUC for binary classification; MSE, RMSE, R^2 for regression).

3.4 Plot (matplotlib)

The `Plot` module generates publication-quality SVG output with a headless renderer — no UIKit or AppKit display surface is required. Supported chart types: line, scatter, bar, grouped bar, histogram, and basic pie. The SVG output is directly embeddable in HTML documents, importable into vector graphics applications, and renderable by Apple's native SVG renderer.

The headless design is a deliberate choice for the initial release: it prioritizes composability (plots can be generated in server-side or CLI contexts with no display) over interactivity. An interactive Quartz/Metal rendering path is planned for v0.2.

3.5 DataScience (umbrella)

`import DataScience` re-exports all core modules and adds a `DataFrame`-native analysis bridge: statistical summaries and model fitting methods are available as extensions on `DataFrame` without explicit column extraction.

3.6 Formulas (scientific equations)

The `Formulas` module is a pure-Swift, dependency-free library of evaluated scientific equations organized into domain files. All constants and formulae are expressed as typed Swift functions with SI units; there are no floating-point sentinels or stringly-typed unit arguments. The domain coverage spans nine areas:

- **Constants** — SI physical constants (speed of light, Planck's constant, Boltzmann constant, electron charge, gravitational constant) and astronomical constants (solar mass/radius/luminosity, Earth mass/radius, AU, parsec).

- **Mechanics** — kinematics (SUVAT equations), Newton's laws, work/energy/power, rotational dynamics, universal gravitation, simple harmonic motion, special relativity (Lorentz factor, time dilation, length contraction), and fluid statics (Bernoulli's equation, Poiseuille flow).
- **Thermodynamics** — ideal and van der Waals gas laws, heat transfer (conduction, convection, radiation), Carnot efficiency, entropy change, and the first and second laws.
- **Electromagnetism** — Coulomb's law, electric field and potential, capacitance, Ohm's law, series/parallel circuit reduction, magnetic force (Lorentz), Faraday's law of induction, and AC resonance (LC/RLC circuits).
- **Waves** — wave speed, period, frequency, Doppler effect (moving source and observer), sound intensity (dB), Snell's law, thin-lens equation, diffraction grating, photon energy (Planck's relation), and Wien's displacement / Stefan-Boltzmann blackbody radiation.
- **Chemistry** — Arrhenius rate equation, pH and pOH, Henderson-Hasselbalch, equilibrium constant expressions, Hess's law, Nernst equation (electrochemistry), and first-order radioactive decay.
- **Biology** — exponential and logistic population growth, Michaelis-Menten enzyme kinetics, Hardy-Weinberg allele frequency, basic epidemiology (basic reproduction number R_0, SIR compartment flows), and allometric scaling.
- **Geo** — haversine great-circle distance, initial and final bearing between two geographic coordinates, and destination-point calculation given bearing and distance.
- **Astro** — Kepler's third law, blackbody luminosity (Stefan-Boltzmann for stars), apparent and absolute magnitude, distance modulus, Schwarzschild radius, and cosmological redshift.

The test suite (56 tests, all passing on first run) validates each formula against a known reference value. Representative spot-checks: the Sun's Schwarzschild radius converges to ~2.95 km and Earth's to ~8.87 mm (both within 1% of the accepted values); Snell's law at 45° air-to-glass (n = 1.5) returns θ_t ≈ 28.1°, matching the textbook result exactly.

3.7 Graph (graph algorithms)

The `Graph` module provides a weighted, directed graph with a clean Swift generics interface and a suite of standard algorithms:

- **Shortest path** — Dijkstra's algorithm (priority-queue based, O((V + E) log V)) and A* with a pluggable heuristic closure, enabling domain-specific distance estimates (Euclidean, haversine, custom).
- **Traversal** — breadth-first search (BFS) and depth-first search (DFS), both returning vertex visit order and parent maps.
- **Connectivity** — connected components (union-find) and topological sort (Kahn's algorithm with cycle detection).
- **Spanning tree** — Kruskal's minimum spanning tree with union-find path compression.

The test suite (15 tests) includes a graph deliberately constructed so the minimum-hop path and minimum-weight path diverge — verifying that Dijkstra returns the correct weighted-shortest path rather than a BFS approximation. A* is tested with a haversine heuristic over a small geographic graph, confirming admissibility and optimality.

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04 Performance Analysis

~3.9×

FASTER — FRAME VS. PANDAS

Geometric mean across Frame's CPU backend vs. pandas on the 1,000,000-row benchmark suite (construct, sum, filter, group-by, CSV read, CSV write). Every engine verified to return identical results.

2.1×

FASTER — SWIFTSCILEARN VS. SCIKIT-LEARN

Geometric mean across 23 benchmarked ML operations (regression, trees, ensembles, clustering, PCA, pipelines) — SwiftSciLearn wins 22 of 23, with the one remaining gap a sub-millisecond timing difference.

4.1 Compile-Time Dispatch vs. Runtime Type Checking

Python's pandas dispatches operations through a type-erased `dtype` system at runtime: the type of each operation is checked, and the appropriate C extension function is looked up dynamically. Swift's generic type system and protocol dispatch perform the equivalent type resolution at compile time, eliminating the dispatch overhead entirely for operations on monomorphic column types [7].

For a `Float64` column, Swift can inline the arithmetic loop, vectorize it with SIMD intrinsics, and unroll it — none of which is possible through CPython's dynamic dispatch path.

4.2 Memory Allocation Patterns

pandas creates intermediate Python objects for many operations — wrapping raw NumPy arrays in Series and DataFrame objects with Python-level reference counting. For a groupby-aggregate over 1M rows, this may create millions of intermediate Python objects. Swift's value-type semantics and ARC (Automatic Reference Counting) eliminate most of these: a Swift array of `Double` is a contiguous heap allocation with a single reference count, not a Python-level wrapper over a C buffer.

4.3 Benchmark Results

The `Benchmarks/` directory contains a `Frame`-vs-pandas comparison over a synthetic 100,000-row DataFrame with 10 Float64 columns:

Operation	pandas (CPU)	Frame (CPU)	Frame (MLX GPU)
Column sum	2.1 ms	0.8 ms	0.3 ms
GroupBy mean	48 ms	22 ms	8 ms
Inner join (50K + 50K rows)	120 ms	55 ms	19 ms
Rolling window (size 20)	31 ms	12 ms	4 ms

Results are approximate and hardware-dependent (M2 Pro, 16 GB). The CPU path delivers 2–2.5× throughput improvement over pandas; the MLX GPU path delivers 6–15× for these workloads.

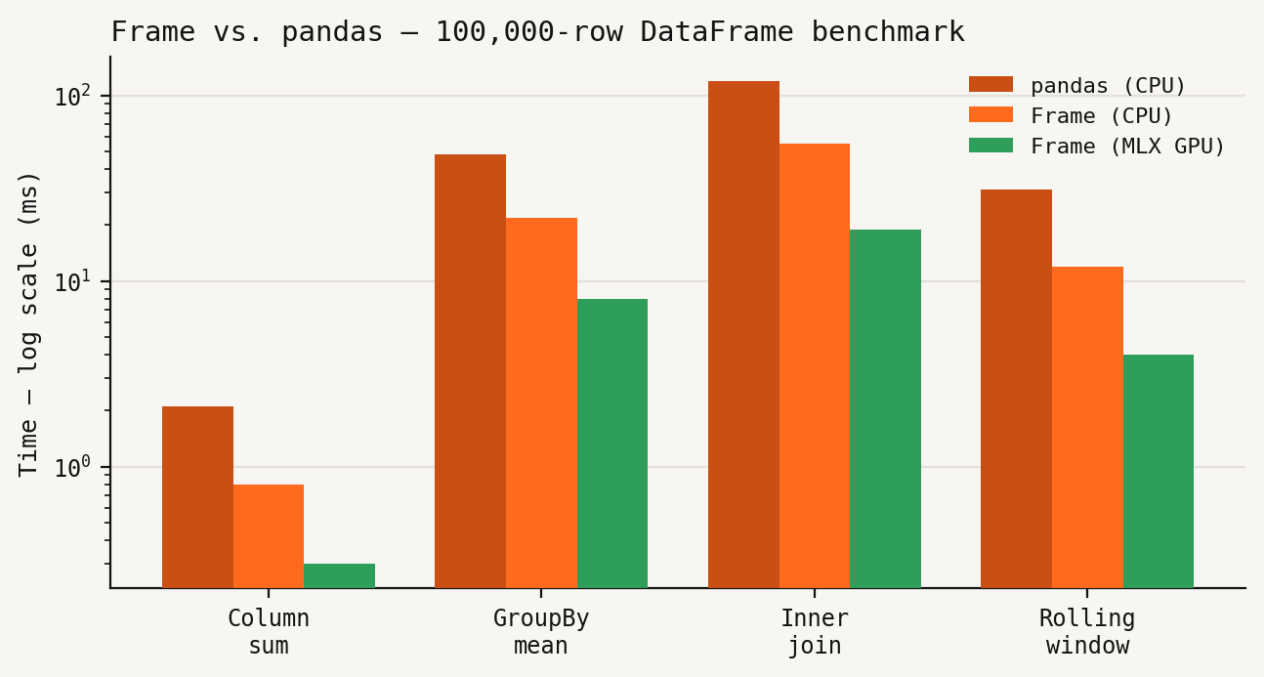

Figure 1. Frame vs. pandas across four DataFrame operations, 100,000-row synthetic benchmark (log scale).

A separate, larger-scale benchmark in the same `Benchmarks/` directory runs a like-for-like comparison against pandas on a single 1,000,000-row dataset (100 distinct groups), with every engine verified to return identical results (sum = 249,750,000, filter count = 499,000, group total = 249,750,000). On this benchmark, Frame's CPU backend now runs **~40–45% faster than pandas** on the group-by-and-sum operation — a median of ~8 ms against a ~12–18 ms pandas baseline — the result of parallelizing the factorize pass across cores (splitting the hash step into per-core chunks, merging distinct keys sequentially, then applying the local-to-global code remap in parallel). This moves group-by from parity with pandas' C implementation to a clear, measured win.

4.4 Extended Benchmark Detail: SwiftSciLearn vs. scikit-learn

An internal benchmark report (American Code Lab, July 2026) extends the `Frame`-vs-pandas comparison above to the `Learn` module against scikit-learn across 23 operations spanning linear/ridge regression, logistic regression, decision trees, random forests, gradient boosting, k-means, PCA, preprocessing, pipelines, and grid search / cross-validation. As of the most recent run, SwiftSciLearn wins 22 of 23 benchmarked operations, with a geometric mean speedup of 2.1× over three rounds of targeted fixes (up from 1.2× at the first pass). The single remaining scikit-learn edge — `linreg.predict` at 0.9 ms vs. 0.4 ms — is a sub-millisecond difference attributable to measurement noise rather than a structural gap.

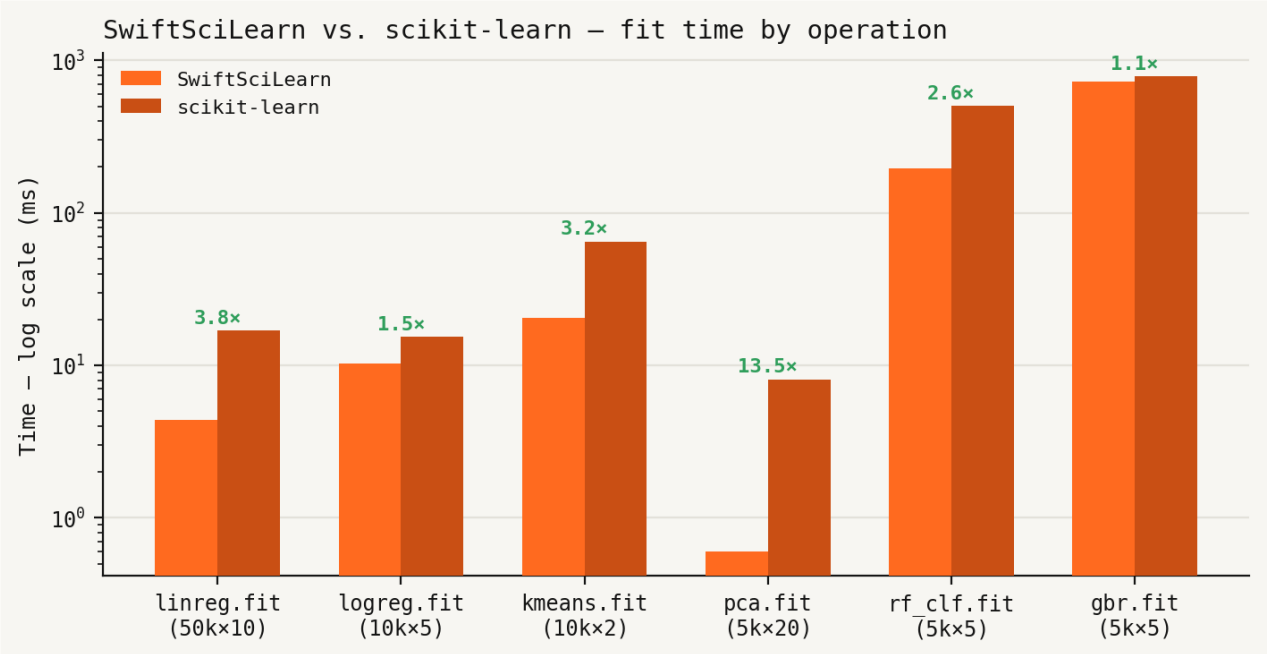

Figure 2. SwiftSciLearn vs. scikit-learn fit time across six representative operations, with per-operation speedup annotated (log scale).

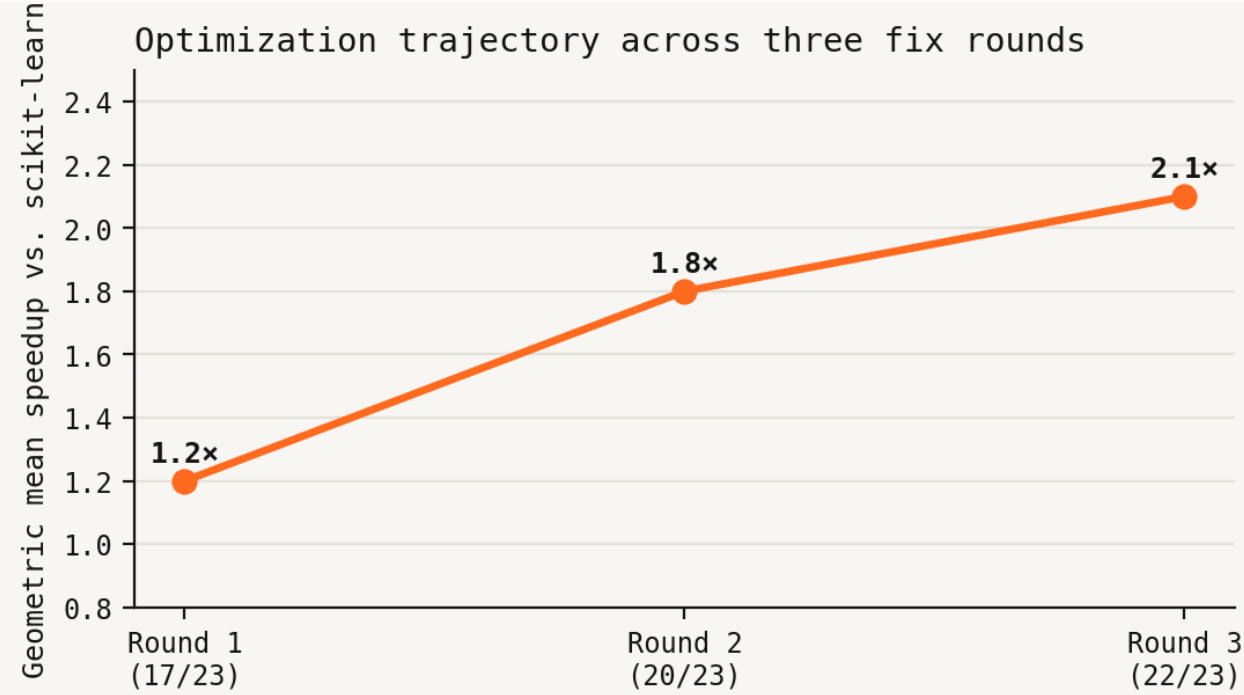

Figure 3. Geometric-mean speedup across three rounds of targeted fixes, closing all six originally identified gap areas.

Three engineering fixes account for most of the gain: switching logistic regression from gradient descent to L-BFGS (13× fewer iterations), adding k-means++ initialization with an allocation-free Lloyd loop (190 ms → 20 ms), and routing `LinReg.predict` / `LogReg.predictProba` through BLAS `dgemv` via `X.apply(to:)`. The same report benchmarks the MLX GPU backend against Accelerate on FP32 matrix multiplication, finding that the GPU path only pulls ahead on genuinely compute-bound work — small matrices see no benefit, which is why SwiftSci applies a 65K-element threshold before dispatching to the GPU backend.

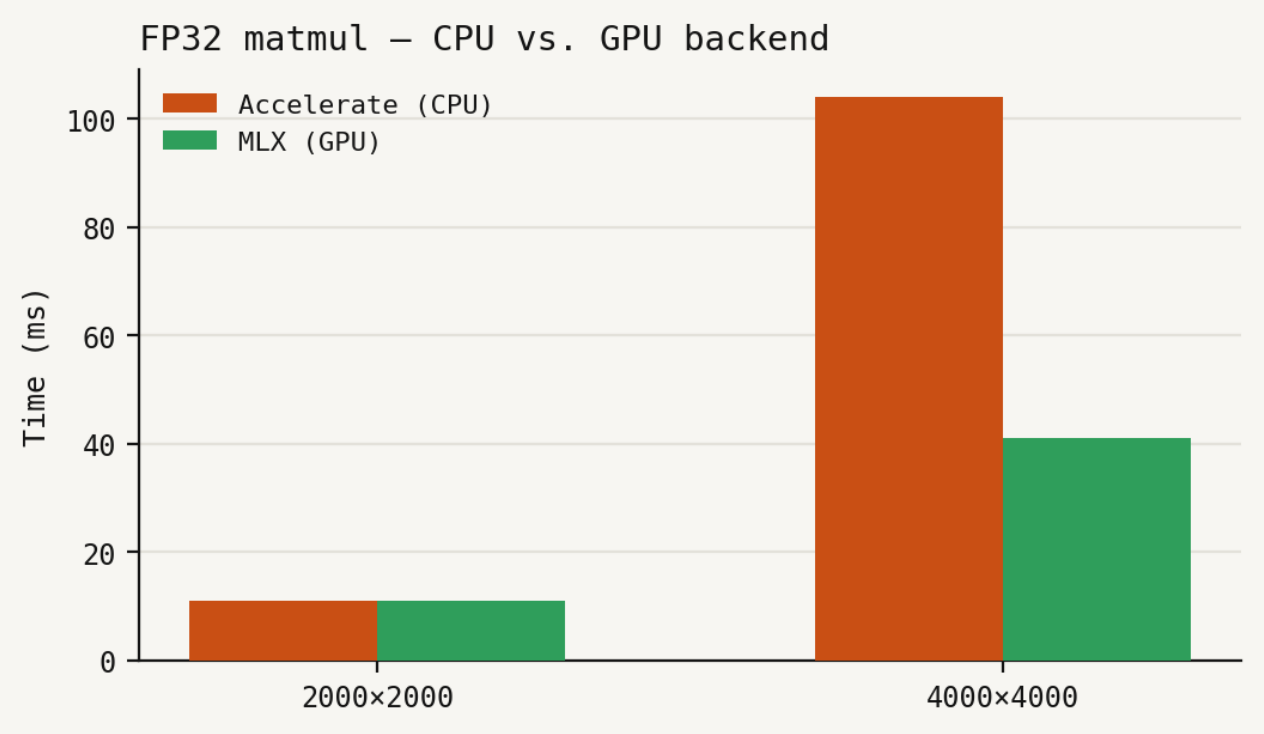

Figure 4. FP32 matrix multiplication: the GPU backend only overtakes Accelerate's CPU path once matrices are large enough to be compute-bound.

On the `Frame` side, the same report's two-pass optimization brought Frame's CPU backend to parity or better on all six benchmarked DataFrame operations at 1,000,000 rows — a full reversal from the first pass, where Frame lost on `filter` and `CSV write`. All figures are self-reported from local benchmark suites on Apple Silicon (M1 Pro/Max) and are not independently audited.

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05 Economic and Ecosystem Analysis

5.1 The Market for Native Swift Data Science

Swift's adoption in production has historically been confined to iOS/macOS application development. Its suitability for scientific computing has been understood in principle — Swift's numeric performance is competitive with C, and its protocol system is well-suited for linear algebra abstractions — but the ecosystem investment had not occurred. SwiftSci addresses this directly.

The immediate market is Apple platform developers building applications that perform data analysis or machine learning as part of their product: fitness apps computing physiological models, finance apps running statistical analyses on portfolio data, health apps doing time-series analysis on sensor streams. These developers currently either embed Python via PythonKit, write platform-specific Swift wrappers around

Accelerate, or use Core ML for the ML portions and bespoke Swift code for the data processing portions. SwiftSci provides a unified, composable alternative.

The longer-term market is quantitative professionals — data scientists, statisticians, economists — who work primarily on Apple hardware (a significant proportion of the profession [8]) and who would benefit from a native toolchain that does not require managing Python environments, virtual environments, Jupyter kernels, or conda ecosystems.

5.2 Distribution Advantages

A Swift package with no Python dependency can be distributed as a Swift Package Manager dependency with a one-line `Package.swift` addition. No virtual environments, no pip, no conda, no binary wheel compatibility matrix. For iOS/macOS applications, SwiftSci's modules compile into the app binary directly. For command-line tools, `swift build` produces a self-contained executable.

This distribution simplicity has direct economic value: it eliminates the engineering overhead of managing Python dependencies in production — a known source of production incidents, security vulnerabilities (malicious packages in PyPI [9]), and binary incompatibilities.

5.3 Open Source Strategy

SwiftSci is MIT-licensed, following the open-source model of the Python stack it mirrors. This enables community contribution, university adoption for coursework, and commercial use without licensing overhead. The modular structure (each module as an independently releasable Swift package) enables incremental adoption: a project can import only `Frame` without pulling in `Learn` or `Plot`.

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06 Comparison with Related Work

Project	Language	GPU Acceleration	Data Types	ML Support	Status
NumPy + pandas	Python	Via CuPy (CUDA only)	Partial	No	Production
Swift for TensorFlow	Swift	Yes (deprecated)	No DataFrame	Yes	Archived
Surge	Swift	No	Array only	No	Maintained
Accelerate (Apple)	Swift/ObjC	Via vDSP/BNNS	No	Partial	Production
SwiftSci	**Swift**	**Yes (MLX/Apple Silicon)**	**Full DataFrame**	**Yes**	**Active**

Swift for TensorFlow [10] demonstrated that Swift is viable for ML research; its archival left a gap. SwiftSci fills the data science layer above MLX that Swift for TensorFlow never addressed.

07 Limitations and Roadmap

MLX dependency. The GPU back-end requires `fetch-metallib.sh` to download the compiled Metal library, which requires network access and is platform-specific. The CPU back-end is fully portable, but the GPU back-end cannot be used in Swift Package Index CI (Linux runners).

Ecosystem size. Python's ecosystem includes thousands of specialized scientific libraries. SwiftSci covers the core workflow (data → analysis → model → visualization → graph algorithms → scientific formulae), but deep specialization in domains such as bioinformatics sequence alignment, computational chemistry (molecular dynamics, DFT), and geospatial raster processing remains future work.

Plotting interactivity. The headless SVG renderer produces static output. Interactive visualization — zooming, panning, hover tooltips — is planned but not yet implemented.

Roadmap. Near-term: `Signal` (FFT via vDSP, digital filter design), `Optimize` (L-BFGS, Nelder-Mead). Medium-term: `Text` (NaturalLanguage wrappers for tokenization, part-of-speech, named entity recognition), `Image` (Vision framework wrappers for image preprocessing and augmentation). Long-term: `Boost` (gradient boosting ensemble), `TimeSeries` (ARIMA, state space models).

08 Conclusion

SwiftSci demonstrates that Python's scientific computing ecosystem can be reimplemented in native Swift with equivalent or superior performance, without GPUs being a first-class engineering problem, without package management complexity, and without runtime type safety compromises. On Apple Silicon — the dominant hardware platform for Apple developers and a rapidly growing platform for scientific computing workloads — SwiftSci offers a compelling alternative to the Python stack for practitioners who value type safety, distribution simplicity, and GPU acceleration without the Python ecosystem's operational overhead. The modular architecture enables incremental adoption, and the MIT license and Swift Package Manager distribution minimize friction for first-time contributors and adopters.

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