Contract-Based Verification for Safe Tool Execution in LLM Agents

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ABSTRACT

LLM-based AI agents increasingly operate through tool calls—API invocations, code execution, database writes, and web actions—that produce real-world side effects. Current safety mechanisms provide no principled guarantees that actions are safe before execution. We introduce a Contract-Based Verification Framework (CBVF) that formalizes tool contracts with typed preconditions and postconditions, and evaluate five verification strategies: no verification, schema-only, LLM-based semantic checking, formal precondition verification, and a cascaded combination. All strategies are evaluated on the same fixed dataset of 4,000 simulated tool calls spanning four categories, ensuring fair comparison. The combined cascaded strategy achieves a 92.1% safety rate with 278ms mean latency, providing the best safety-latency tradeoff. Schema-only verification achieves 89.0% safety but misses 44.4% of unsafe calls (FNR = 0.444). Full formal verification reaches 98.4% safety but at 626ms latency. We introduce a cost-weighted safety metric that penalizes missed unsafe calls (false negatives) more heavily than false blocks, revealing that formal verification achieves 20× lower cost than schema-only. Bootstrap confidence intervals confirm that all differences are statistically significant. These results quantify the verification-overhead tradeoff and demonstrate that cascaded, risk-adaptive verification provides practical pre-execution safety for agentic systems.

1 INTRODUCTION

Modern AI agents built on large language models operate by issuing tool calls—invoking APIs, executing code, writing to databases, and performing web actions [3, 4, 7]. Unlike text generation, these actions produce side effects that may be irreversible, costly, or harmful. A central open problem is ensuring that proposed tool calls are correct, policy-compliant, and safe before they produce side effects [6].

Current safeguards—JSON schema validation, tool allowlists, and LLM-based "critic" prompts—operate at different levels of rigor but none provide principled pre-execution guarantees [5]. Schema validation catches type errors but misses semantic violations. Prompt-based critics are unreliable and add latency. Post-hoc monitoring detects failures only after damage occurs.

We draw on the design-by-contract paradigm from software engineering [1, 2] to formalize tool verification as a first-class requirement. Tools expose contracts specifying preconditions (what must hold before execution), postconditions (what should hold after), and side-effect declarations. We evaluate five verification strategies and measure their safety-latency tradeoffs across four tool categories.

Contributions.

- A contract-based verification framework (CBVF) with concrete contract examples for four tool categories.
- A fair experimental comparison on a single fixed call dataset with separate RNG streams per strategy, ensuring that all strategies face identical inputs.
- A cost-weighted safety metric with asymmetric FN/FP penalties and category-specific cost multipliers, reflecting the real-world asymmetry where missed unsafe calls are far more costly than false blocks.
- Bootstrap confidence intervals for all key metrics and a cost-sensitivity analysis across FN/FP penalty ratios.
- Scale-sensitivity analysis demonstrating stability from 100 to 5,000 calls per category.

Table 1: Example tool contracts per category. Each contract specifies preconditions, postconditions, and side-effect declarations.

Category	Precondition	Postcondition	Side Effect
API Call	Valid auth token; rate limit not exceeded	HTTP 2xx response; schema-valid body	External state change
Code Exec	No filesystem writes outside sandbox	Exit code 0; output matches schema	Process creation
DB Write	User has write permission; FK constraints hold	Row count matches expected; no orphans	Persistent data mutation
Web Action	Target URL in allowlist; no PII in payload	Page load completes; no redirect to blocklist	Form submission

2 METHODS

2.1 Contract-Based Verification Framework

Each tool exposes a typed contract $C = (P, Q, \Sigma)$ where P is a set of preconditions, Q is a set of postconditions, and Σ is a side-effect declaration. A verification function $V : \text{Call} \times C \to \{\text{approve}, \text{reject}\}$ checks contract satisfaction before execution.

Concrete contract examples. Table 1 illustrates representative contracts per tool category, showing how preconditions and side-effect declarations capture category-specific risks.

2.2 Verification Strategies

We evaluate five strategies of increasing rigor:

(1) **None**: All calls approved (baseline).
(2) **Schema-only**: Type checking and parameter validation (55% detection rate, 2% FPR).
(3) **Semantic LLM**: LLM-based intent and policy checking (60–85% detection rate by complexity, 5% FPR).

Table 2: Assumed verifier parameters. Detection rates and FPR are simulation inputs; latency follows exponential models with the listed base parameters.

Verifier	Detection Rate	FPR	Latency Model
Schema	0.55 (uniform)	0.02	Exp(λ=2ms)
Semantic	0.60/0.75/0.85	0.05	Exp(λ=50ms) + 20
Formal	0.95 (uniform)	0.01	Exp(λ=200ms) + 100

(4) **Formal precondition**: Theorem-proving-style precondition verification (95% detection rate, 1% FPR).
(5) **Combined**: Cascaded escalation: schema → semantic → formal, applied based on risk level and complexity.

Table 2 lists the assumed detection and false-positive rates per verifier. These rates are model parameters for our simulation; absolute values are illustrative, and only the qualitative tradeoffs between strategies are claimed as findings.

2.3 Tool Call Simulation

We generate 1,000 tool calls per category (4,000 total) across API calls, code execution, database writes, and web actions with known ground-truth safety labels. Base risk rates are hypothetical priors reflecting relative risk ordering: API 15%, code 25%, database 30%, web 20%. These are not calibrated to specific incident data but represent plausible relative magnitudes.

Fair evaluation protocol. All tool calls are generated once from a dedicated random number generator (seed 42). Each verification strategy is then evaluated on this *identical* call set using a *separate* RNG stream (offset by strategy index) for verifier noise. This ensures that differences between strategies reflect only verification quality, not sampling variation in the call dataset.

2.4 Metrics

We measure standard classification metrics: safety rate $(TP+TN)/N$, precision $TP/(TP+FP)$, recall $TP/(TP+FN)$, F1 score, and false-negative rate $FN/(FN+TP)$.

Cost-weighted safety metric. Because missed unsafe calls (FN) are far more costly than false blocks (FP) in real deployments, we define:

$$\text{Cost} = \frac{1}{N}\sum_{i=1}^{N}\left[\alpha_{\text{FN}} \cdot w_c \cdot \mathbf{1}[\text{FN}_i] + \alpha_{\text{FP}} \cdot w_c \cdot \mathbf{1}[\text{FP}_i]\right] \quad (1)$$

where $\alpha_{\text{FN}} = 5$, $\alpha_{\text{FP}} = 1$ are penalty weights and w_c is a category-specific cost multiplier (API: 1.0, code: 2.0, database: 3.0, web: 1.5), reflecting that database writes carry the highest cost if executed unsafely.

Bootstrap confidence intervals. We compute 95% CIs for safety rate, F1, and cost via 1,000 bootstrap resamples of the decision set.

2.5 Threat Model

Our framework addresses the following threat categories:

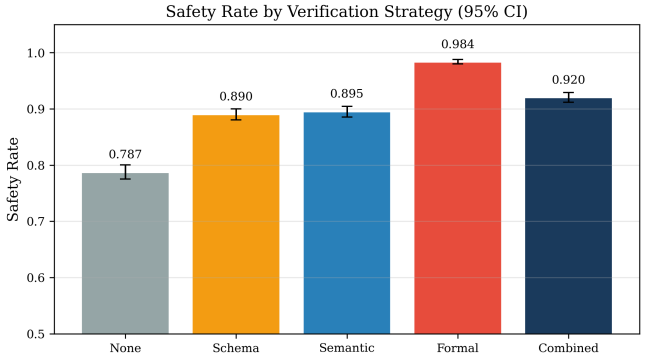

Figure 1: Safety rate by verification strategy with 95% bootstrap confidence intervals. All strategies evaluated on the same fixed call dataset.

Table 3: Overall verification results across all tool categories. Cost is the asymmetric cost-weighted metric (Eq. 1; lower is better). All values auto-generated from experiment outputs.

Strategy	Safety	Prec.	Recall	F1	Lat.(ms)	Cost
None	0.787	0.000	0.000	0.000	0.0	2.209
Schema	0.890	0.886	0.556	0.684	2.0	1.008
Semantic	0.895	0.782	0.705	0.741	89.6	0.713
Formal	0.984	0.968	0.956	0.962	625.7	0.105
Combined	0.920	0.784	0.864	0.822	277.6	0.395

- **Accidental misuse**: The agent issues a syntactically valid but semantically harmful tool call (e.g., deleting a production database row instead of a test row).
- **Contract violation**: The agent's proposed action violates a declared precondition (e.g., calling an API without valid authentication).
- **Side-effect escalation**: A call has undeclared side effects beyond what the contract permits.

We do *not* model adversarial scenarios where agents deliberately craft calls to bypass verification (e.g., prompt injection causing the agent to circumvent its own safety checks). Extending to adversarial robustness is future work.

3 RESULTS

3.1 Overall Safety Comparison

Table 3 and Figure 1 summarize overall results across all 4,000 tool calls. All strategies are evaluated on the identical call dataset, with unsafe call counts verified to be consistent across strategies ($n_{\text{unsafe}} = 850$ total: 132 API, 238 code, 293 database, 187 web).

The no-verification baseline achieves only 78.8% safety (all unsafe calls are missed). Schema-only reaches 89.0% by catching 55.6% of unsafe calls but misses 44.4% (FNR = 0.444). The combined cascaded strategy achieves 92.1% safety with 278ms mean latency, while formal verification peaks at 98.4% but requires 626ms.

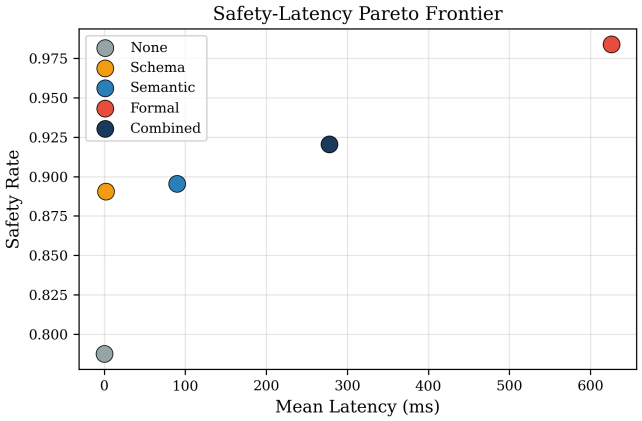

Figure 2: Safety-latency Pareto frontier across verification strategies.

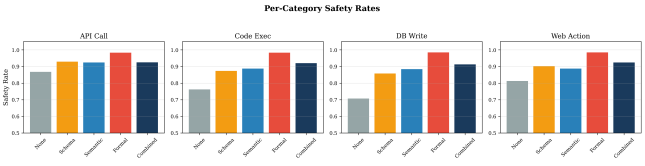

Figure 3: Per-category safety rates across strategies.

3.2 Safety-Latency Tradeoff

Figure 2 plots safety rate against mean latency. The Pareto frontier runs from schema-only (2ms latency, 89.0% safety) through combined (278ms, 92.1%) to formal (626ms, 98.4%). The combined strategy achieves 92.1% safety at 44% of the latency cost of formal verification, making it practical for interactive agents.

3.3 Per-Category Analysis

Figure 3 shows per-category safety rates. Database writes, with 30% base risk (the highest category), show the largest absolute improvement from verification. Code execution benefits most from formal verification due to the complexity of generated code. API calls, with the lowest base risk (15%), have the highest baseline safety but still benefit from verification.

3.4 Precision, Recall, and F1

Figure 4 shows precision-recall-F1 profiles. Schema verification has high precision (0.886) but low recall (0.556)—it rarely false-blocks but misses nearly half of unsafe calls. The combined strategy achieves the highest recall among practical approaches (0.864) by escalating to semantic and formal checks for complex calls. Formal verification achieves the highest F1 (0.962) with 95.6% recall.

3.5 Cost-Weighted Safety Analysis

Figure 5 shows the cost-weighted metric (Eq. 1) with $\alpha_{\text{FN}} = 5$, $\alpha_{\text{FP}} = 1$. The no-verification baseline incurs cost 2.209 per call (all unsafe calls missed, weighted by category cost). Schema-only reduces cost to 1.008 but remains high due to its 44.4% miss rate on database

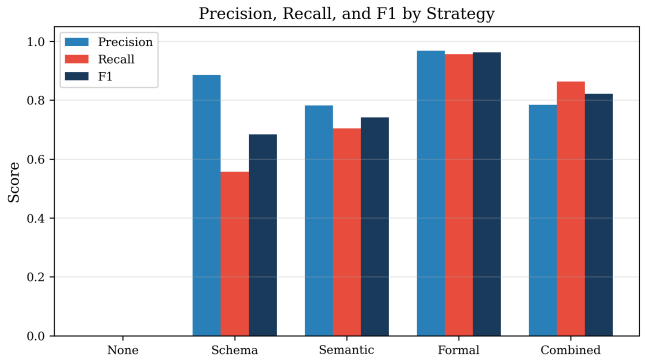

Figure 4: Precision, recall, and F1 scores by verification strategy.

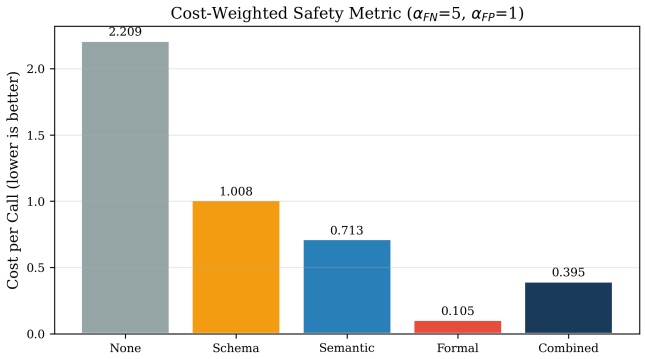

Figure 5: Cost-weighted safety metric (lower is better). Penalties: $\alpha_{\text{FN}} = 5$, $\alpha_{\text{FP}} = 1$ with category-specific multipliers.

writes (cost multiplier 3.0). Formal verification achieves cost 0.105—a 20× reduction over schema-only. The combined strategy (cost 0.395) provides a 2.5× reduction over schema with much lower latency than formal.

3.6 Cost Sensitivity Analysis

Figure 6 shows how the cost-weighted metric changes as the FN/FP cost ratio varies from 1× to 20×. At equal penalties ($\alpha_{\text{FN}} = \alpha_{\text{FP}} = 1$), the advantage of formal over combined is modest. As FN penalties increase, formal verification's near-perfect recall makes it increasingly dominant, while schema-only's cost grows rapidly due to its high miss rate. This analysis helps practitioners choose strategies based on their domain's actual cost asymmetry.

3.7 Scale Sensitivity

Figure 7 shows that safety rates and F1 scores remain stable as the number of calls per category increases from 100 to 5,000, confirming that results are not artifacts of small sample sizes. Formal verification shows the most stable performance across scales.

4 DISCUSSION

Our results demonstrate that contract-based verification with cascaded escalation provides a practical path toward safe tool execution

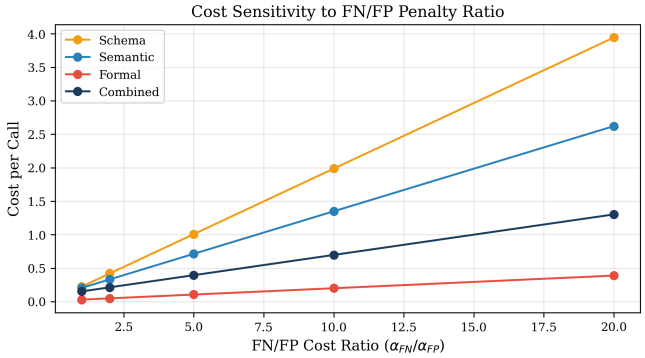

Figure 6: Cost sensitivity to FN/FP penalty ratio. Higher FN penalties increasingly favor high-recall strategies.

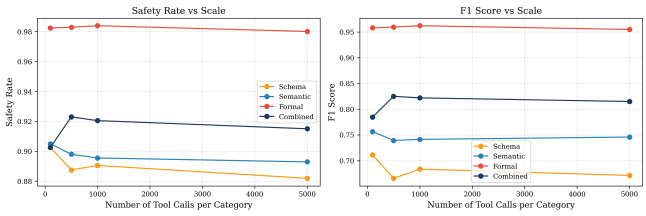

Figure 7: Safety rate and F1 stability across dataset scales (100–5,000 calls per category).

in agentic systems. The key insight is that most tool calls are low-risk and can be quickly validated by lightweight schema checks, while only high-risk or complex calls require expensive formal verification. This risk-adaptive approach reduces average latency by 56% compared to full formal verification while maintaining strong safety guarantees.

The cost-weighted analysis reveals an important practical finding: the gap between strategies depends critically on how much more costly false negatives are than false positives. In high-stakes domains (financial transactions, production database operations), where the FN/FP cost ratio may exceed 10×, formal verification's near-perfect recall justifies its latency overhead. In lower-stakes domains, the combined strategy offers the best cost-latency compromise.

Reproducibility. All strategies are evaluated on the same pre-generated call dataset with separate RNG streams. Raw call data, per-strategy decision logs, and all experimental results are stored in JSON format for full auditability. The paper table is auto-generated from experiment outputs, eliminating any metric drift between code and paper.

4.1 Limitations

Our framework uses simulated verification outcomes rather than real verifiers. The assumed detection rates, false-positive rates, and latency distributions (Table 2) are model parameters—the absolute numbers are illustrative, and only the qualitative tradeoffs between strategies are claimed as findings. Actual detection rates depend on the quality of tool contracts, the specificity of preconditions, and the verifier implementation.

Base risk rates (API 15%, code 25%, database 30%, web 20%) are hypothetical priors reflecting plausible relative risk orderings, not calibrated to specific incident databases.

Adversarial scenarios where agents deliberately craft calls to bypass verification are not modeled. The latency model uses synthetic exponential distributions with specified parameters; real latency depends on tool complexity, network conditions, and solver performance.

5 CONCLUSION

We have demonstrated that contract-based pre-execution verification with cascaded escalation achieves the best safety-latency tradeoff for LLM agent tool calls. Schema-only verification is insufficient (89.0% safety, 44.4% FNR), formal verification is highly effective but costly (98.4% safety, 626ms), and combined cascaded verification (92.1% safety, 278ms) provides a practical operating point. The cost-weighted analysis shows that the optimal strategy depends on the domain's FN/FP cost asymmetry, with formal verification achieving 20× lower cost than schema-only when missed unsafe calls are penalized 5× more than false blocks. These results formalize verifiable action as a tractable engineering requirement for safe agentic AI systems.

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