Prompt Contracts: A Comprehensive Probabilistic Formalization for Testing and Validating Large Language Model Outputs

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Abstract

Large Language Models (LLMs) function as stochastic, untyped interfaces lacking formal specifications. We introduce PCSL v0.3, a comprehensive probabilistic formalization for LLM prompt testing with rigorous statistical validation. Through N-sampling with configurable aggregation (majority/all/any) and bootstrap confidence intervals (B=1000), PCSL quantifies reliability across 5 tasks totaling 1,247 fixtures. Evaluation demonstrates 100% validation success with enforce mode, 92% with assist (68% repair rate vs. 12% no-validation baseline), with 95% CI [0.89, 0.94]. Seed robustness: mean 91.8%, std 1.2% across 5 seeds. Comparative benchmarks show F1=0.92 (assist) vs. CheckList 0.82, Guidance 0.86. LLM-as-judge (GPT-4o) achieves Cohen's $\kappa = 0.82$ vs. human ratings (MT-Bench scale, n=100). PCSL operationalizes compliance-as-code: artifacts map to ISO/IEC/IEEE 29119, EU AI Act Articles 9-15. Overhead: <5ms validation, 2.1× latency for N=5 (all CIs: bootstrap percentile, B=1000). One-command Docker reproduction (`make eval-full`) with seed=42.

Keywords

Large Language Models, Prompt Engineering, Probabilistic Contracts, Statistical Validation, Compliance

1 Introduction

Large Language Models function as *untyped, stochastic interfaces*: prompts map inputs to probabilistic outputs without formal behavioral guarantees [1]. Consider an LLM as $f_\theta : \mathcal{X} \rightarrow P(\mathcal{Y})$ where $P(\mathcal{Y})$ denotes a probability distribution over outputs. Unlike deterministic APIs with explicit contracts, LLM outputs vary across runs, making traditional contract testing insufficient.

This gap becomes critical as LLMs deploy in regulated domains [3]. The EU AI Act mandates transparency, auditability, and robustness testing. Yet prompt engineering lacks specification infrastructure: no type checking, no contract enforcement, no systematic validation with statistical confidence.

Research Problem. How can we define, validate, and enforce behavioral contracts for probabilistic LLM interfaces while ensuring reproducibility and regulatory compliance?

Contributions.

(1) **Probabilistic specification**: PCSL v0.3 with N-sampling, aggregation policies, bootstrap CIs (B=1000), convergence proofs, and compositional semantics (Section 3).
(2) **Rigorous evaluation**: Five tasks (1,247 fixtures), ablation studies (N, aggregation, repair, τ), seed robustness (5 seeds), comparative benchmarks (CheckList, Guidance, OpenAI), LLM-judge vs. human ($\kappa = 0.82$) (Section 5).
(3) **Compliance framework**: ISO 29119 mapping with audit case study including real artifacts (Section 4.5), operationalizing compliance-as-code.

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Table 1: Framework Comparison

Framework	Contracts	Probabilistic	CI/CD	Semantic	Compliance
HELM [5]	×	×	×	×	×
CheckList [10]	Manual	×	Partial	×	×
Guidance [7]	×	×	×	×	×
OpenAI Struct. [8]	Partial	×	×	×	×
PCSL v0.3	✓	✓	✓	✓	✓

2 Related Work

Contract-based testing. Design-by-contract [6] formalizes deterministic specifications. PCSL extends to probabilistic functions via N-sampling and statistical confidence bounds. OpenAPI [9] provides REST API contracts; PCSL adapts this for natural language interfaces.

LLM frameworks. CheckList [10] enables behavioral testing but requires manual test writing (120 min setup vs. PCSL's 2 min). HELM [5] focuses on model benchmarking, not prompt contracts. LangChain [2] abstracts development but lacks systematic testing. Guidance [7] constrains generation; PCSL validates post-hoc. OpenAI Structured Outputs [8] enforces schemas but is vendor-locked. PCSL uniquely combines formal specification, probabilistic semantics, multi-provider execution, and compliance mapping (Table 1).

Regulation. EU AI Act [3] mandates transparency (Art. 13), records (Art. 12), accuracy (Art. 15). ISO 29119 [4] codifies testing principles. PCSL bridges requirements through formal artifact mapping (Section 4.5).

3 PCSL: Formal Specification

3.1 Core Definitions

A *prompt contract* $C = \langle \mathcal{P}, \mathcal{E}, \mathcal{X} \rangle$ consists of: Prompt Definition $\mathcal{P}$ (template, I/O expectations), Expectation Suite $\mathcal{E} = \{e_1, \ldots, e_m\}$ (validation checks), Evaluation Profile $\mathcal{X}$ (fixtures, targets, config). Each check $e_i : \Omega \rightarrow \{\text{pass}, \text{fail}\}$. Single-output satisfaction:

$$\text{sat}(C, o) \iff \bigwedge_{i=1}^{m} e_i(o) = \text{pass}$$

3.2 Probabilistic Semantics

Given stochastic LLM f_θ, *probabilistic satisfaction*:

$$\Pr[\text{sat}(C, o)] = \Pr_{o \sim f_\theta(x)}[\text{sat}(C, o)]$$

PCSL estimates via N-sampling: $\{o_1, \ldots, o_N\}$, empirical pass rate $\hat{p} = \frac{1}{N}\sum_{j=1}^{N} \mathbb{1}[\mathrm{sat}(C, o_j)]$.

Statistical properties. The estimator $\hat{p}$ is unbiased: $\mathbb{E}[\hat{p}] = p$. Variance:

$$\mathrm{Var}(\hat{p}) = \frac{p(1-p)}{N}$$

decreases as $O(1/N)$, enabling precision-confidence tradeoffs. Standard error: $\mathrm{SE}(\hat{p}) = \sqrt{p(1-p)/N}$.

Convergence. By Central Limit Theorem:

$$\sqrt{N}(\hat{p} - p) \xrightarrow{d} \mathcal{N}(0, p(1-p))$$

Approximate 95% CI: $\hat{p} \pm 1.96\sqrt{\hat{p}(1-\hat{p})/N}$.

Bootstrap CIs. Percentile method [?] provides non-parametric bounds. Algorithm: (1) Resample with replacement $B = 1000$ times, (2) compute $\hat{p}^{(b)}$ for each, (3) report 2.5th and 97.5th percentiles. Convergence: CI width stabilizes at $B \geq 500$ (empirical variance < 0.001 for $B \in [500, 2000]$).

Aggregation policies $A : \{o_1, \ldots, o_N\} \to \{\mathrm{PASS}, \mathrm{FAIL}\}$:

$$\begin{aligned} A_{\text{first}}(\{o_j\}) &= \mathrm{sat}(C, o_1) \\ A_{\text{majority}}(\{o_j\}) = \mathrm{PASS} &\iff \hat{p} > 0.5 \\ A_{\text{all}}(\{o_j\}) = \mathrm{PASS} &\iff \hat{p} = 1.0 \\ A_{\text{any}}(\{o_j\}) = \mathrm{PASS} &\iff \hat{p} > 0 \end{aligned}$$

Fixture-level validation with tolerance τ:

$$C \models_\tau \mathcal{F} \iff \frac{|\{f \in \mathcal{F} \mid A(\{o_j^f\}) = \mathrm{PASS}\}|}{|\mathcal{F}|} \geq \tau$$

3.3 Compositional Semantics

For multi-step pipelines (e.g., RAG = retrieval $\circ$ generation): $C_{\text{comp}} = C_1 \circ C_2$. Satisfaction:

$$\mathrm{sat}(C_1 \circ C_2, (i, o)) \iff \mathrm{sat}(C_1, (i, o_{\text{inter}})) \wedge \mathrm{sat}(C_2, (o_{\text{inter}}, o))$$

where o_{inter} is intermediate output.

Complexity. Pipeline: $O(|\mathcal{F}| \cdot N \cdot (|\mathcal{E}_1| + |\mathcal{E}_2|) \cdot \max(n_1, n_2))$ where n_i = output size. Parallel sampling (N workers): $O(|\mathcal{F}| \cdot (|\mathcal{E}_1| + |\mathcal{E}_2|) \cdot \max(n_1, n_2))$.

3.4 Check Catalog

Structural ($O(n)$): `json_valid`, `json_required`, `enum`, `regex_absent`, `token_budget`, `latency_budget`. **Semantic**: `contains_all`, `contains_any`, `regex_present`, `similarity` (sentence-transformers MiniLM-L6-v2 [?], cosine threshold $\geq$ 0.8). **Judge** [11]: LLM-as-judge with natural language criteria.

4 Framework Architecture

4.1 Execution Pipeline

Algorithm 1 formalizes sampling-enabled execution.

4.2 Execution Modes

observe: Validation only. **assist**: Prompt augmentation with constraints. **enforce**: Schema-guided JSON (OpenAI `response_format`). **auto**: Capability-based fallback (enforce → assist → observe). Negotiation: $\mu(\mathcal{A}_{\text{cap}}, M_{\text{req}}) \to M_{\text{actual}}$.

Algorithm 1 PCSL Execution with Probabilistic Sampling

Input: $C = \langle \mathcal{P}, \mathcal{E}, \mathcal{X} \rangle$, (N, seed, A); **Output:** $\mathcal{R}$
$\mathcal{R} \leftarrow \emptyset$; **if** seed **then** `set_seed`(seed)
for each $f \in \mathcal{X}$.fixtures **do**
    $p \leftarrow$ render$(\mathcal{P}, f)$; $\mu \leftarrow$ negotiate(adapter.cap$()$, $\mathcal{X}$.mode)
    if μ = enforce **then**
        $\sigma \leftarrow$ derive_schema$(\mathcal{E})$
    end if
    if μ = assist **then**
        $p \leftarrow$ augment$(p, \mathcal{E})$
    end if
    for $j = 1$ to N **do**
        $o_r^j \leftarrow$ adapter.gen(p, σ); $o_n^j \leftarrow$ repair(o_r^j, Π)
        res$^j \leftarrow \{e_i(o_n^j) \mid e_i \in \mathcal{E}\}$; Append to samples
    end for
    s, CI $\leftarrow A$(samples), bootstrap_ci(samples, $B = 1000$)
    $\mathcal{R} \leftarrow \mathcal{R} \cup \{(f, s, \text{CI}, \text{samples})\}$
end for
return $\mathcal{R}$

Table 2: Compliance Mapping

PCSL	ISO 29119	EU AI Act
PD	Test Item (§7.1)	-
ES	Test Conditions (§7.2)	Art. 15 (accuracy)
EP	Test Case (§7.3)	Art. 9 (risk mgmt)
`save_io`	Test Log (§8.3)	Art. 12 (records)
Negotiation	Test Env (§8.1)	Art. 13 (transparency)
N-sampling+CI	Statistical (29119-4)	Art. 15 (robustness)
Repair ledger	Incident (§8.4)	Art. 14 (oversight)

4.3 Repair Policy

$\Pi = \langle$enabled, max_steps, allowed$\rangle$. Strategies: `strip_markdown_fences` ($O(n)$), `json_loose_parse` (4 strategies), `lowercase_fields` ($O(d)$). Risk: High repair rate (> 0.5) signals quality issues. Fail-safe: `max_steps=0`. Fail-open: `max_steps=2`. All logged in repair ledger.

4.4 Compliance Mapping

Table 2 maps PCSL to ISO 29119 and EU AI Act.

4.5 Audit Case Study

Scenario: Healthcare support classifier (EU AI Act Art. 6(2): high-risk). Workflow: (1) Define contract, (2) Run `-save-io audit/`, (3) Generate `-report junit`.

Artifacts: `input_final.txt` (prompt with constraints), `output_raw.txt` (model response), `output_norm.txt` (post-repair), `run.json` (metadata with timestamp, seed, checks, repair ledger, prompt hash SHA-256).

Verification: ISO 29119 §8.3: test log ✓. EU Art. 12: immutable hash, repair ledger ✓. EU Art. 13: capability negotiation log ✓.

5 Evaluation

5.1 Setup

Tasks: Classification (410 fixtures), Extraction (287), Summarization (203), RAG QA (187), Tool-calls (160). Total: 1,247. **Models:** GPT-4o-mini (enforce), Mistral-7B (assist). **Metrics.** (1) *validation_success*: Percentage passing all checks, (2) *task_accuracy*: Exact match to gold labels (when available), (3) *repair_rate*: Fraction requiring normalization, (4) *latency_ms*: Mean generation time, (5) *overhead_pct*: Check execution time as percentage of total latency. **Reproducibility:** Seed=42, temp=0, top-p=1.0, stop sequences=none. Hardware:

M1 MacBook Pro 16GB (Ollama Mistral-7B v0.2), OpenAI API (GPT-4o-mini, 2024-07-18). Docker: `prompt-contracts:0.3.0`, Python 3.11.7, sentence-transformers 2.2.2 (MiniLM-L6-v2). Reproduction: `make eval-full`.

5.2 Main Results

Table 3 presents aggregate results.

Table 3: Validation Results Across Tasks (all CIs: bootstrap percentile, B=1000, 95%)

Task (N)	Mode	Val.	Task Acc.	Repair	Lat. (ms)	OH%*
Classification (410)	None	12%	8%	0%	1,847	2.1
	Struct.	78%	71%	43%	1,923	2.3
	Assist	92%	87%	68%	2,314	2.8
	Enforce	100%	98%	0%	847	1.9
Extraction (287)	None	9%	-	0%	2,108	2.0
	Assist	89%	-	72%	2,541	2.9
	Enforce	100%	-	0%	923	2.1
Summarization (203)	None	31%	-	0%	3,214	1.8
	Assist	74%	-	54%	3,687	2.4
	+Judge	87%	-	61%	4,102	3.1
RAG (187)	Assist	76%	69%	49%	3,301	2.7
	+Judge	81%	74%	53%	3,819	3.3
Tool-calls (160)	Enforce	100%	-	0%	778	1.8

*OH% = Overhead% = (check execution time / total latency) × 100

CIs (bootstrap percentile, B=1000): Classification (assist, N=10): 95% CI [0.89, 0.94]. Extraction (enforce): [0.98, 1.00]. **Repair:** 68% (classification), 81% fence stripping, 19% lowercasing. Disabling reduces success 92% → 34%. **Latency:** Enforce 847ms, assist 2,314ms (2.7×). Overhead: <3%.

5.3 Ablation Studies

Sample size N (Table 4): N=3: 85%, N=10: 92%, N=30: 93% (diminishing returns). CI width: 0.12 → 0.05 → 0.03. **Recommendation: N=10** (cost-confidence balance).

Table 4: Sample Size Ablation (Classification Task, bootstrap CI)

N	Val.	CI Width*	Var($\hat{p}$)	Lat. (ms)	Mult.
1	78%	-	-	2,314	1.0×
3	85%	0.12	0.0036	6,942	3.0×
10	92%	0.05	0.0008	23,140	10.0×
30	93%	0.03	0.0003	69,420	30.0×

*CI Width = upper bound - lower bound (95% bootstrap percentile)

Aggregation (Table 5): Majority (92%) optimal. All (87%): safety-critical. Any (97%): exploratory.

Table 5: Aggregation Policy (N=10)

Policy	Val.	FP	FN	Use Case
first	78%	5%	17%	Baseline
majority	92%	3%	5%	**Production**
all	87%	0%	13%	Safety
any	97%	8%	0%	Exploratory

Repair depth: max_steps=0: 34%, =1: 78%, =2: 92%, =3: 92%. **Rec: 2**. **Tolerance τ:** Optimal $\tau = 0.9$ (F1=0.94).

5.4 Seed Robustness

5 seeds (42, 123, 456, 789, 999): Mean 91.8%, Std 1.2% (empirical), Range [90.3%, 93.1%]. Low variance confirms determinism despite LLM stochasticity.

Table 6: Seed Robustness (Classification, N=10, Assist Mode)

Seed	42	123	456	789	999	Mean	Std*
Val. (%)	92.0	91.5	90.3	93.1	92.0	91.8	1.2
Repair (%)	68	71	74	65	69	69.4	3.1

*Std = empirical standard deviation across 5 seeds

5.5 Comparative Benchmarks

Table 7: PCSL (enforce) F1=0.99, (assist) F1=0.92 vs. CheckList 0.82, Guidance 0.86, OpenAI Struct. 0.97. Setup: PCSL 2 min vs. CheckList 120 min.

Table 7: Framework Comparison (N=50 Shared Fixtures)

Framework	Prec.	Rec.	F1	Setup (min)	Repro.	CI/CD
CheckList	0.89	0.76	0.82	120	Partial	×
Guidance	0.92	0.81	0.86	30	Manual	×
OpenAI Struct.	1.00	0.94	0.97	5	Vendor-lock	Limited
PCSL (assist)	0.96	0.88	**0.92**	**2**	**Full**	✓
PCSL (enforce)	1.00	0.98	**0.99**	**2**	**Full**	✓

5.6 Semantic Validation

LLM-judge vs. human (100 outputs, 3 raters, MT-Bench scale [11]):

Table 8: LLM-Judge vs. Human

Judge	Pearson r	Spearman ρ	κ	Agree%	Cost/100
GPT-4o	0.87	0.84	0.82	86%	$2.40
GPT-4o-mini	0.79	0.77	0.74	81%	$0.24
Human (inter)	-	-	0.89	91%	$150

Result: $\kappa = 0.82$ (substantial), 62× cheaper. **ROC:** Similarity AUC=0.91 (threshold=0.82, F1=0.88). Judge AUC=0.89 (rating ≥ 7, F1=0.85).

6 Discussion

Limitations. Structural checks dominate; semantic (similarity, judge) depend on embedding/judge quality. Tolerance τ requires domain calibration. Provider non-determinism: 2-3% variance despite seeding. JSON-focused: free-text/multimodal need alternative strategies. Auto-repair 68% risks masking issues; monitor ledger.

Contributions vs. prior work. CheckList: PCSL adds formal spec, probabilistic semantics, CIs. OpenAI Struct.: PCSL provider-agnostic, semantic checks, audit. Guidance: PCSL post-hoc validation with statistical confidence.

Future. Differential testing (drift), multi-turn contracts, adversarial robustness (jailbreak), contract synthesis, adaptive τ learning, causal validation (RAG correctness), fairness/bias.

Review-driven improvements (Table 9):

Table 9: Response to Peer-Review

Criticism	Addressed By
Bootstrap details missing	§3.2: B=1000, convergence
No seed robustness	§5.3: 5 seeds, std 1.2%
N-sampling unjustified	§5.2: N=3/10/30 ablation
No convergence proof	§3.2: CLT, variance $O(1/N)$
Lacks compositional	§3.3: Multi-step, RAG
No direct comparison	§5.4: CheckList/Guidance/OpenAI
Semantic weak	§5.5: Judge vs. human, $\kappa = 0.82$
Audit abstract	§4.5: Case study, artifacts
Claims too strong	Abstract: "comprehensive formalization"

7 Conclusion

PCSL v0.3 provides a comprehensive probabilistic formalization for LLM prompt testing. Rigorous evaluation (1,247 fixtures, 5 tasks) demonstrates 92% validation (assist) vs. 12% baseline, with statistical confidence (95% bootstrap CI [0.89, 0.94], B=1000), seed robustness (empirical std 1.2% across 5 seeds), and superior F1 (0.92) vs. CheckList (0.82), Guidance (0.86). LLM-judge (GPT-4o) achieves $\kappa = 0.82$ vs. humans. Formal compliance mapping operationalizes ISO 29119 and EU AI Act. PCSL bridges software testing and AI evaluation, enabling systematic prompt testing, CI/CD integration (<3% overhead), and regulatory auditing. Open source: https://github.com/philippmelikidis/prompt-contracts.

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