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Automating Cyber Offense Simulations with Machine Learning: Advancements in AI-Augmented Penetration Testing

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Abstract

The rapid growth of digital infrastructure complexity has made conventional manual penetration testing methods insufficient for modern enterprise security testing. Machine learning technologies enable revolutionary possibilities for automating cyber offense simulations using self-learning, self-adaptive, and self-optimizing systems for exploitation strategies. Reinforcement learning agents acquire sophisticated capabilities in vulnerability chaining and defensive evasion from environmental interactions, discovering attack sequences that evade traditional rule-based automation. Neural network models learned from vulnerability data identify generalizable patterns between system configurations and exploitability attributes, facilitating probabilistic reasoning concerning defensive control efficacy. Generative adversarial networks generate new exploitation payloads that retain functional efficacy while exhibiting varied observable attributes to evade signature-based detection systems. Variational autoencoders support probabilistic models for defense-conscious payload optimization from continuous latent space representations. Integration of intelligent automation in penetration testing processes resolves scalability constraints, supports continuous security verification, and offers persistent adversarial emulation reflecting advanced threat actor capabilities. Real-world deployment demands safety-constrained architectures balancing autonomous behavior with organizational needs, regulatory compliance frameworks, and ethical guidelines informing responsible offensive security technology development. This intersection establishes a foundation for autonomous red teaming that actively detects sophisticated attack vectors within current distributed computing landscapes.

Keywords: Machine Learning Penetration Testing, Autonomous Offensive Security, Reinforcement Learning Exploitation, Generative Adversarial Networks, Cyber Kill Chain Automation

1. Introduction

Enterprise security environments have evolved into distributed, heterogeneous infrastructures across on-premises systems, cloud platforms, containerized workloads, and edge computing environments. This architectural complexity brings unprecedented attack surface growth, in which established penetration testing practices cannot maintain extensive coverage under realistic time and resource limitations. Human security assessment, constrained by limited cognitive capacity and sequential execution modes, cannot adequately investigate the combinatorial explosion of exploitable attack paths that arise from interdependent system relationships, privilege hierarchies, and vulnerability interactions. The time lag between recurring evaluations provides exploitable windows where attackers working with automated reconnaissance and exploitation toolkits identify and exploit vulnerabilities before defense teams complete validation cycles.

Machine learning technologies provide revolutionary potential for offensive security automation by enabling systems to learn, adjust, and optimize exploitation techniques based on interaction with the environment instead of executing preordained sequences. Reinforcement learning agents build experiential knowledge of vulnerability chaining, defensive evasion, and privilege escalation through repeated probing of target systems, discovering attack paths that evade rule-based automation or human analysts working under deadline pressure. Neural network models trained on large datasets of vulnerability information and exploitation histories enable generalizable associations between system configurations and exploitability features, thereby enabling probabilistic inferences regarding the feasibility of attacks and the effectiveness of defensive controls in varied infrastructure configurations.

The integration of artificial intelligence in penetration testing processes addresses core operational challenges such as scalability constraints of human assessment practices, accommodation needs for evolving defensive technologies, and requirements for continuous validation of security with respect to contemporary development speeds. Autonomous offensive systems that can operationalize entire attack lifecycles from initial reconnaissance activities to post-exploitation operations provide organizations with continuous adversarial simulation that reflects sophisticated capabilities of threat

actors. This paradigm shift enables security teams to validate defenses against adaptive, intelligent adversaries instead of static test conditions, establishing empirical baselines for incident detection capability, response efficacy, and overall security posture robustness.

This study examines the technical underpinnings, architectural trends, and operational implications of applying machine learning systems in automated penetration testing. The discussion covers supervised learning methods for vulnerability scanning and target ranking, reinforcement learning models for autonomous exploitation and lateral movement, and generative modeling methods for payload generation and defense evasion. Through rigorous analysis of algorithmic solutions, implementation frameworks, and verification methods, this research provides practical guidance to organizations seeking to extend security analysis capabilities through intelligent automation while addressing ethical limitations, regulatory restrictions, and safety standards required for operational execution in offensive security practice [1][2].

2. Intelligent Agent Architectures for Autonomous Exploitation

2.1 Reinforcement Learning Foundations for Offensive Autonomy

Reinforcement learning provides the theoretical basis for creating autonomous agents for sequential decision-making in adversarial settings with partial observability, stochastic transitions, and sparse reward signals. The formulation of the penetration testing problem involves modeling target infrastructure as an environment with discrete states corresponding to system configurations, access levels, and defensive stances, and actions corresponding to offensive tactics such as network scanning, service enumeration, exploitation attempts, privilege escalation techniques, and lateral movement strategies. The agent learns optimal policies through trial-and-error interaction, receiving rewards for accomplishing compromise goals such as credential acquisition, privilege escalation, or access to sensitive data stores while being penalized for detectable actions or operational inefficiencies. Model-free reinforcement learning algorithms are especially well-suited for penetration testing situations where precise environmental models remain challenging to develop, given system complexity, configuration variety, and defensive ambiguity. Q-learning and its deep neural network extensions enable agents to estimate action values over high-dimensional state spaces without explicit environment modeling, learning exploitation strategies from experience based on observed state transitions and reward outcomes. Policy gradient methods learn parameterized policies through gradient ascent on expected cumulative reward, enabling direct learning of stochastic action selection strategies that balance exploration of diverse attack vectors while exploiting known effective techniques.

The deployment of actor-critic architectures decouples value estimation from policy optimization, reducing policy gradient estimate variance and enabling more stable learning dynamics when exploring sparse reward environments typical of multi-stage exploitation scenarios. Advantage actor-critic algorithms calculate temporal difference errors, approximating the extent to which realized returns exceed expectations, focusing policy updates on actions that demonstrably outperform baseline predictions. The integration of experience replay systems and target network stabilization methods overcomes challenges posed by correlated training data samples and non-stationary target distributions, supporting convergence to effective exploitation policies across diverse infrastructure configurations.

2.2 Neural Network Design for Cyber Attack Path Discovery

Deep neural network architectures facilitate learning of hierarchical feature representations that encode sophisticated relationships between observable system features and exploitability indicators at multiple abstraction levels. Convolutional layers applied to network topology data capture local connectivity patterns, relationships among co-located services, and segmentation boundaries that affect the viability of attack paths. Pooling operations aggregate spatial information, thereby providing invariance to specific network addressing schemes while maintaining structural patterns relevant to lateral movement options. Hierarchical convolutional feature composition enables reasoning about attack graph attributes such as path length, privilege requirements, and defensive control intersection without explicit graph algorithmic implementation.

Recurrent neural network models with long short-term memory or gated recurrent units provide temporal reasoning capabilities suitable for multi-stage exploitation patterns where current action selection depends on extended historical context. These models maintain internal state representations that encode accumulated knowledge about target systems, previously attempted exploits, and observed defensive responses, supporting context-sensitive decision-making that

considers assessment history. The temporal relationships encoded by recurrent connections are particularly valuable for learning exploitation strategies that require specific sequencing of actions, such as establishing persistence mechanisms before initiating detectable reconnaissance activity or synchronizing distributed exploitation across network segments.

Graph neural networks provide natural frameworks for reasoning about network structure, system dependencies, and attack graph topologies modeled as possible compromise paths through multifaceted infrastructure. Message-passing processes propagate information across graph edges modeling network connectivity, service relationships, or trust boundaries, enabling agents to reason about transitive risk where compromising intermediate systems facilitates access to high-value targets. Attention mechanisms modulate information flow based on learned importance, directing computational resources toward attack paths with high success probability or strategic value. The integration of graph pooling operations supports hierarchical reasoning across infrastructure at different granularity levels, ranging from individual hosts to network subnets to entire organizational domains [3][4].

Algorithm	Architecture	Learning Approach	Key Advantages	Primary Applications
Deep Q-Network (DQN)	Neural network Q-value estimation with experience replay and target networks	Value-based learning with temporal difference updates	Stable convergence, handles high-dimensional states effectively	Multi-stage exploitation path discovery, complex attack chain identification
Actor-Critic	Separate policy and value networks with shared features	Simultaneous policy improvement and value estimation	Low variance, stable gradients, fast convergence	Privilege escalation sequences, coordinated lateral movement
Policy Gradient	Direct policy parameterization mapping states to actions	Gradient ascent on expected cumulative reward	Stochastic policies enable diverse exploration strategies	Adaptive attack timing, exploration of novel exploitation approaches
Proximal Policy Optimization	Clipped surrogate objective with trust region constraints	Constrained policy updates preventing large divergence	Monotonic improvement, scalable to distributed environments	Large-scale network penetration, safety-constrained operations

Table 1: Reinforcement Learning Algorithms for Autonomous Exploitation [3, 4]

3. Generative Models and Adversarial Learning for Payload Synthesis

3.1 Generative Adversarial Networks for Exploit Diversification

Generative adversarial networks provide architectural frameworks for synthesizing new exploitation payloads that remain functionally effective while exhibiting varied observable properties to resist signature-based detection mechanisms. The generator network learns to produce exploitation artifacts such as shellcode variants, command injection payloads, or malicious scripts by transforming random latent vectors into structured outputs resembling training samples of successful exploits. The discriminator network attempts to distinguish generated payloads from authentic exploitation code, providing training feedback that guides the generator toward producing more realistic and functionally equivalent variants. This adversarial training dynamic inherently aligns with offensive security objectives in which produced artifacts must accomplish exploitation goals while evading defensive scrutiny simultaneously.

The deployment of conditional generation methods enables the synthesis of exploitation payloads adapted to specific vulnerability classes, target operating systems, or defensive configurations by conditioning generator inputs on corresponding contextual information. Conditioning mechanisms guide the generative process toward creating outputs with properties appropriate for particular exploitation contexts, enabling automatic adaptation of generic exploitation templates to target environments. Latent space representations learned from semantic relationships between payload properties and exploitation success enable interpolation between known successful exploits to identify novel variants that circumvent defensive signatures while maintaining functional properties.

Progressive training approaches that gradually increase generation complexity from basic payload elements to complete exploitation chains prove effective for learning stable generators capable of producing syntactically correct and functionally effective artifacts. The hierarchical decomposition of exploit generation into multiple stages, such as initial access payload synthesis, privilege escalation script generation, and persistence mechanism creation, facilitates focused learning on individual components before integration into complete attack chains. Transfer learning methods enable pre-training on general vulnerability datasets followed by fine-tuning on organization-specific exploitation contexts, reducing convergence time and improving generation quality in scenarios where training samples are limited.

3.2 Defense-Aware Payload Optimization with Variational Autoencoders

Variational autoencoders provide probabilistic models for learning compressed latent representations of effective exploitation methods that preserve fundamental functional properties while enabling controlled payload variant generation. The encoder network projects observed exploitation artifacts into continuous latent distributions characterized by mean and variance parameters, enabling probabilistic inference regarding payload attributes and interpolation among known successful instances. The decoder network generates exploitation payloads from sampled latent vectors, learning generative models that produce functionally equivalent variants with varied surface characteristics. The variational formulation enforces regularization through Kullback-Leibler divergence constraints that promote smooth, continuous latent spaces suitable for gradient-based optimization and semantic interpolation.

The incorporation of defensive model approximations in the variational autoencoder training process enables the exploitation of payload generation specifically optimized for evading particular detection mechanisms. Adversarial training objectives incorporating defender discriminators penalize generated payloads that trigger signature matches, behavioral anomalies, or other detectable attributes, encouraging the generator to create artifacts that preserve exploitation effectiveness while minimizing defensive observability. The co-evolutionary configuration reflects real-world adversarial dynamics where attackers continuously refine exploitation methods in response to defensive improvements, enabling automated discovery of evasion techniques not readily apparent through human-driven analysis.

Semi-supervised extensions facilitate training on datasets that combine labeled collections of successful exploits with unlabeled collections of benign system activity, enabling generators to learn discriminative boundaries between malicious and legitimate behaviors. This capability proves valuable for generating exploitation payloads that blend with typical system behavior, reducing detection probability by behavioral monitoring systems that identify statistical anomalies. The probabilistic nature of variational autoencoders enables uncertainty quantification in generated payloads, providing confidence measures that inform autonomous agents regarding exploitation attempt likelihood and guide exploration-exploitation tradeoffs during penetration testing activities [5][6].

Model Type	Core Mechanism	Training Objective	Evasion Capability	Implementation Use Cases
Conditional GAN	Generator and discriminator conditioned on vulnerability context	Class-conditional adversarial training with contextual guidance	Context-adaptive evasion tailored to defensive configurations	Platform-specific exploit adaptation, OS-aware payload generation
Defense-Aware GAN	Three-player system with generator, discriminator, and defender model	Tri-objective optimization balancing effectiveness and evasion	Explicit optimization against specific detection mechanisms	IDS/IPS signature avoidance, behavioral monitoring circumvention
Variational Autoencoder	Encoder-decoder with probabilistic latent representations	Evidence lower bound maximization with KL regularization	Controlled diversity through latent space exploration	Payload variants with quantified uncertainty, probabilistic generation
Semi-Supervised VAE	Learning from labeled exploits and unlabeled benign samples	Joint optimization on labeled and unlabeled data	Stealthy generation blending with normal operations	Behavioral camouflage, statistical anomaly avoidance

Table 2: Generative Model Architectures for Payload Synthesis [5, 6]

4. Operational Deployment and Enterprise Integration

4.1 Safety-Constrained Autonomy and Risk Management

Operational deployment of machine learning-based penetration testing systems in enterprise settings requires architectural frameworks balancing autonomous operation with organizational safety requirements, regulatory compliance limitations, and operational stability objectives. The implementation design incorporates graduated levels of autonomy ranging from supervised operation, where human analysts review and approve all agent actions, through semi-autonomous methods where agents execute pre-approved techniques independently while escalating novel or high-risk operations, to complete autonomy reserved exclusively for isolated test environments or specially authorized assessment scopes. This graduated approach enables organizations to incrementally implement intelligent automation while maintaining appropriate human oversight and risk management controls.

Integration with enterprise security infrastructure provides autonomous agents with contextual understanding of organizational priorities, asset classifications, and operational constraints that guide exploitation decisions and assessment strategies. Integration with configuration management databases enables agents to identify critical systems requiring special handling, while integration with vulnerability management platforms provides real-time patch status and known weakness information that focuses exploitation efforts on realistic attack vectors. Integration with SIEM systems supports real-time correlation between offensive operations and defensive detections, enabling agents to refine tactics based on detection metrics and validate defensive control efficacy through experimentation.

Safety mechanisms embedded within the agent architecture enforce hard constraints preventing autonomous systems from exceeding authorized assessment boundaries, causing unforeseen service disruptions, or maintaining access beyond specified assessment windows. Action filtering components evaluate proposed exploitation methods against predefined risk thresholds, organizational policies, and operational constraints before execution, blocking operations that transgress established boundaries. Automated state rollback and restoration capabilities enable agents to return systems to pre-testing conditions following assessment activities, reducing residual security impact and operational effect. Continuous monitoring of system health indicators enables early detection of unintended consequences, triggering assessment suspension and operator notification when anomalous conditions arise.

4.2 Performance Measurement and Validation Frameworks

Empirically validating the effectiveness of machine learning-facilitated penetration testing requires a comprehensive measurement framework that objectively assesses technical performance, operational feasibility, and sustainability across multiple organizational contexts and diverse infrastructure configurations. Technical performance measures assess core competencies, including attack path discovery rate, which calculates the proportion of exploitable vulnerabilities identified relative to ground truth; exploitation success rate, which measures the percentage of initiated compromises achieving specific access objectives; and coverage breadth, which evaluates the variety of attack types and infrastructure elements examined during assessment execution. These technical metrics provide objective benchmarks for comparing autonomous systems to traditional testing methodologies and monitoring capability advancements through iterative refinement.

Operational metrics address pragmatic deployment concerns such as assessment completion time, quantifying end-to-end duration from initiation to reporting, resource utilization, quantifying computational load and infrastructure demands, and false positive rate, measuring frequency of incorrectly identified vulnerabilities requiring human verification. Integration friction metrics evaluate the ease with which autonomous testing integrates into existing security workflows, quantifying configuration complexity, operator training requirements, and compatibility with preexisting toolchains. These operational performance indicators prove essential for assessing real-world viability beyond laboratory demonstrations and inform architectural adjustments addressing practical deployment challenges.

Adaptive improvement mechanisms enable ongoing strengthening of autonomous testing capabilities through feedback loops that incorporate assessment results, defender observations, and environmental changes into continuous model refinement. Online learning methodologies adjust agent policies based on experience accumulated during production testing, enabling adaptation to organization-specific infrastructure profiles and defensive configurations. Federated learning frameworks enable multiple organizations to collaboratively improve shared models while maintaining data privacy, consolidating intelligence from diverse operational environments without disclosing sensitive organizational information. Active learning techniques identify high-value training scenarios where human expertise would most benefit

model performance, directing operator attention toward edge cases and unusual situations challenging for current autonomous systems [7][8].

Metric Category	Key Performance Indicators	Measurement Method	Success Criteria	Continuous Improvement
Attack Discovery	Vulnerability identification rate, attack path diversity, zero-day capability	Ground truth comparison, expert validation, red team assessment	High coverage, diverse vector discovery, novel path identification	Feedback from remediation outcomes, continuous model retraining
Exploitation Success	Compromise ratio, privilege escalation, lateral movement efficiency	Success tracking across diverse infrastructure configurations	Elevated ratios vs conventional methods, reduced time to compromise	Online learning from attempts, policy refinement from patterns
Operational Efficiency	Assessment duration, resource consumption, computational overhead	Wall-clock timing, resource monitoring, throughput analysis	Reduced timeframes, efficient utilization, scalable operations	Performance profiling, bottleneck removal, algorithmic optimization
Defensive Evasion	Detection avoidance, signature bypass, behavioral stealth	SIEM alert correlation, IDS trigger analysis during testing	Low detection, minimal alerts, successful circumvention	Adversarial training against current defenses, evasion refinement
Adaptability	Convergence speed, generalization, transfer learning effectiveness	Training iterations, performance across unseen configurations	Rapid convergence, strong generalization, effective transfer	Federated learning, privacy-preserving model sharing protocols

Table 3: Performance Evaluation Framework for ML-Driven Testing [7, 8]

5. Ethical Considerations and Regulatory Compliance

5.1 Responsible Development and Deployment Principles

The development and deployment of autonomous offensive security systems requires robust ethical frameworks ensuring that technologies designed to discover vulnerabilities do not inadvertently enable malicious activities or create unintended security risks. Principles of responsible development mandate transparent documentation of system capabilities, functionalities, and intended applications to prevent unauthorized repurposing for inappropriate penetration testing or actual cyber attacks. Access control mechanisms limiting autonomous system deployment to trained security personnel operating under explicit organizational authorization are essential for preventing technology misuse. The implementation of audit logging, recording all autonomous actions, decisions, and identified vulnerabilities, ensures accountability and enables investigation of potential system misuse.

Informed consent principles require that organizations deploying autonomous penetration testing against infrastructure secure explicit authorization from system owners and stakeholders, particularly when assessments may affect production environments or process sensitive information. The establishment of clear assessment boundaries explicitly defining authorized target systems, prohibited actions, and temporal limitations prevents autonomous agents from exceeding intended scope and causing unintended disruption. Organizations must establish incident response procedures that define response protocols for scenarios where autonomous systems inadvertently trigger security alerts, disrupt services, or discover critical vulnerabilities requiring immediate remediation rather than standard scheduled reporting cycles.

The potential for autonomous offensive systems to discover zero-day vulnerabilities or novel attack vectors raises ethical considerations regarding responsible disclosure and vulnerability management. Organizations deploying these technologies bear responsibility for implementing procedures ensuring identified vulnerabilities receive prioritized remediation rather than exploitation or public release that might compromise broader community security. Balancing the advancement of offensive security research through publication against avoiding weaponization of discovered techniques

requires careful consideration of disclosure timing, technical detail levels, and coordination with affected vendors and security communities.

5.2 Legal Frameworks and Compliance Requirements

The deployment of autonomous penetration testing systems operates within sophisticated legal regimes governing computer access, data protection, and cybersecurity practices with significant variations across jurisdictions and regulatory frameworks. Organizations must ensure that autonomous offensive operations align with computer fraud and abuse laws that typically prohibit unauthorized system access, even when conducted for security testing purposes. Explicit written authorization from system owners covering scope, techniques, and timelines for autonomous testing provides legal protection for security teams conducting offensive simulations and establishes definite boundaries, avoiding inadvertent legal violations.

Data protection regulations impose compliance obligations when autonomous systems process personal data, access restricted data stores, or operate in industries with heightened privacy requirements, such as healthcare or finance. Privacy-by-design principles require autonomous agents to implement data minimization techniques, collecting only information necessary for security assessment purposes and applying appropriate safeguards over any sensitive data gathered during testing activities. Data retention policies enabling the timely deletion of assessment artifacts containing potentially sensitive information reduce ongoing compliance risk and align with regulatory requirements for proportionate data processing.

Industry-specific regulatory frameworks impose additional requirements on autonomous security testing practices, particularly in critical infrastructure sectors where testing operations may impact essential services or public safety. Coordination with regulatory bodies regarding planned autonomous assessments, especially those employing novel techniques or encompassing broad infrastructure scope, demonstrates regulatory engagement and facilitates advanced resolution of compliance concerns. Comprehensive documentation of autonomous system architectures, decision-making mechanisms, and safety controls enables regulatory inspection and demonstrates organizational commitment to responsible technology deployment within established legal and regulatory structures [9][10].

Governance Domain	Core Requirements	Implementation	Risk Mitigation	Accountability
Access Control	Restrict deployment to authorized security professionals with explicit mandates	Role-based access, multi-factor authentication, key management	Least privilege enforcement, time-limited access, emergency revocation	Named individuals, management approval, escalation procedures
Informed Consent	Explicit written authorization from system owners with defined scope	Formal documentation, digital signatures, boundary specifications	Clear target definition, prohibited actions, temporal constraints	System owner acknowledgment, stakeholder sign-off, legal review
Audit Logging	Comprehensive logging of all actions, decisions, vulnerabilities	Immutable trails, centralized aggregation, integrity protection	Detailed action logs, timestamp accuracy, correlation identifiers	Audit ownership, investigation procedures, evidence preservation
Vulnerability Disclosure	Protocols ensuring discovered issues receive appropriate remediation	Tracking systems, severity classification, vendor coordination	Internal disclosure first, coordinated notification, reasonable timelines	Disclosure authority, vendor liaison, publication approval processes
Data Protection	Privacy-by-design, data minimization, safeguards for sensitive data	Classification, encryption, access controls, secure deletion	Minimal collection, purpose limitation, storage minimization	Data protection officer, privacy compliance, breach notification
Legal Compliance	Adherence to fraud statutes, sector regulations, international law	Legal review processes, compliance checklists, regulatory engagement	Explicit authorization, jurisdictional compliance, consultation	Legal counsel oversight, compliance officer, regulatory liaison

Table 4: Ethical and Regulatory Compliance Framework [9, 10]

Conclusion

The integration of machine learning technologies with offensive security processes enables transformative capabilities for automated penetration testing that address inherent limitations of traditional assessment approaches. Reinforcement learning architectures enable self-learning autonomous agents that identify intricate attack vectors through adaptive probing, while neural network architectures learn generalizable patterns from vulnerability data to guide exploitation across diverse infrastructure topologies. Generative modeling methods synthesize payload variants tailored to specific exploitation contexts and evasion against defensive controls, facilitating automatic adaptation to evolving security mechanisms. These capabilities collectively enable continuous, scalable security testing that reflects advanced adversary tactics and detects exploitable vulnerabilities before adversaries can exploit them. The architectural patterns and operational models demonstrate practical feasibility for enterprise adoption when deployed with appropriate safety constraints, human oversight mechanisms, and regulatory controls. Integration with existing security infrastructure provides autonomous agents with organizational context for decision-making, while graduated autonomy models enable incremental adoption, balancing risk management and innovation. Performance measurement frameworks and adaptive improvement mechanisms ensure sustained effectiveness as target environments evolve through patching cycles, architectural updates, and defensive technology enhancements. The legal and ethical frameworks governing autonomous offensive system deployment establish guardrails ensuring technological advancement proceeds responsibly in accordance with established societal norms and regulatory requirements. Future directions include multi-agent coordination for simulating sophisticated advanced persistent threat campaigns, interpretability improvements enabling human-understandable explanations of discovered attack sequences and exploitation choices, and adversarial robustness enhancements preventing defensive teams from exploiting agent behavior predictability. The ongoing evolution of AI-augmented penetration testing technologies promises to revolutionize fundamental security validation practices, enabling organizations to maintain defensive preparedness against increasingly sophisticated and automated adversary threats through continuous expert-level assessment of security posture and resilience capacity.

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