Supplementary Materials

Table 1. Characteristics of Sources of Evidence.

First Author	Year	Publication Type	Study Type	Country	AI Technique	QKD Security Focus
H. A. Al-Mohammed	2024	Journal Article	Simulation-Based	Qatar	Autoencoder	Enhancing error correction and scalability for high-data-rate QKD environments.
W. Wang	2020	Thesis	Experimental & Theoretical	Canada	Neural Networks	Optimizing QKD parameters in free-space environments with atmospheric turbulence.
S. R. Sihare	2024	Journal Article	Experimental & Theoretical	India	Error Prediction	Improving error resilience against signal noise and imperfections in guided/unguided QKD.
K. Durak	2022	Journal Article	Experimental	Turkey	Deep Neural Network (DNN)	Detecting side-channel RF fingerprints for physical security of QKD.
M. Ahmadian	2022	Journal Article	Experimental	Spain	DNN for SOP Prediction	Reducing QBER and enhancing Key Exchange Rate in polarization encoded QKD.
M. Nozari	2024	Journal Article	Experimental & Theoretical	UAE & Turkey	DNN	Optimizing underwater QKD under intersymbol interference and background noise.
T. Johann	2023	Conference Proceedings	Simulation-Based	Germany	LSTM Neural Network	Optimizing routing and reducing denial-of-service rates in meshed QKD networks.
H. Zhang	2022	Journal Article	Simulation-Based	China	Autoencoder	Compensating for nonlinear distortion in high-speed CV-QKD.
R. M. Bommi	2023	Conference Proceedings	Experimental & Simulation	India	Various ML Techniques	Enhancing QKD resilience against noise and quantum attacks[4] .

P. Mehdizadeh	2024	Journal Article	Simulation-Based	Iran & Spain	KNN, NN, XGB	Optimizing frequency selection for QKD in multi-band optical transmission.
B. Colombier	2023	Journal Article	Experimental & Theoretical	France	Random Forest	Analyzing power consumption vulnerabilities relevant to QKD security.
J. Xu	2024	Journal Article	Experimental & Theoretical	China	Random Forest	Detecting device imperfections and eavesdropping threats in QKD.
J. Y. Liu	2019	Journal Article	Experimental	China	LSTM Neural Network	Real-time phase modulation stabilization in QKD.
Zi. Ren	2021	Journal Article	Experimental & Theoretical	China	RF, SVM, CNN	Dynamically selecting optimal QKD protocols based on security needs.
Y. Mao	2020	Journal Article	Experimental & Theoretical	China	Artificial Neural Network	Detecting quantum attacks in CV-QKD by analyzing pulse variations.
J. L. Kang	2023	Journal Article	Experimental & Theoretical	China	Various Neural Networks	Optimizing parameter generation rates in Twin-Field QKD[20] .
Y. Yi	2021	Conference Proceedings	Experimental & Theoretical	China	Improved Random Forest	Enhancing transmission probability and optimizing signal strength.
W. Wang	2019	Journal Article	Experimental & Theoretical	China	Feedforward Neural Network	Enhances QKD performance by optimizing parameters for secure and efficient key generation.
Hong-fu Chou	2024	Journal Article	Experimental & Theoretical	Luxembourg	GMM, Bayes Classifier	Detecting Trojan-horse attacks with risk-aware ML in QKD networks[21] .
Hua-Jian Ding	2020	Journal Article	Experimental & Theoretical	China	Random Forest	QKD parameter prediction to optimize secure key generation rates

Table 2. Data Charting Form. Variables and Definitions.

Variable	Definition/Description
Study Details	Information about each study, including:
- First Author	Name of the first author or lead researcher in the study.
- Year	Year of publication.
- Publication Type	Type of publication (e.g., journal article, conference proceedings, thesis).
Machine Learning (ML) Technique	Type of ML algorithms used in the study (e.g., neural networks, random forests) and their purpose in QKD security.
QKD Security Applications	Security challenges addressed by ML, such as mitigating side-channel attacks, noise reduction, or error rate optimization.
Outcome Metrics	Metrics reported to measure effectiveness, including accuracy, response time, adaptability, and scalability.
Country of Study	Country where the research was conducted, typically based on author affiliations.
Study Type	Classification of the study approach, such as simulation-based, experimental, theoretical, or a combination.

Table 3. Sample Data Charting Form Entry.

Study Details	ML Technique	QKD Security Applications	Outcome Metrics	Country	Study Type
Author: Hasan Abbas Al-Mohammed	Autoencoder	Enhancing error correction in high-data-rate QKD	Accuracy > 99%, scalability	Qatar	Simulation-Based
Year: 2024	Neural Networks	Optimizing QKD parameters in free-space	Adaptability to environmental factors	Canada	Experimental & Theoretical

Table 4. Outcomes of Individual Sources of Evidence.

First Author & Year	ML Technique Applied	QKD Security Challenge Addressed	Outcome Metric(s)	Key Findings	Limitations	Future Work
Hasan Abbas Al-Mohammed, 2024	Autoencoder for nonlinear compensation	Error correction, scalability, high data rates, resource optimization in QKD systems	Prediction accuracy > 99%, MSE 17%	Improved QBER and key rate prediction accuracy with scalability benefits	Memory limitations; high computational needs	Integrate with decoy-state methods, apply to different QKD protocols
Wenyuan Wang, 2020	Neural network for parameter	Atmospheric turbulence, channel asymmetry in	2-4 orders of magnitude speedup in parameter optimization	Enhanced efficiency and key rate under asymmetric	Limited real-world testing, dependency on simulation data	Explore multi-user QKD networks; extend to free-space QKD

	optimization	free-space QKD		channel conditions		implementations
Shyam R. Sihare, 2024	Error prediction model	Quantum error resilience, noise impact, signal processing in guided and unguided media	QER prediction accuracy	Improved system robustness through accurate error prediction	Reliance on theoretical models; need for experimental validation	Adaptive error correction techniques; ML-based error prediction for system adjustments
Kadir Durak, 2022	Deep Neural Network (DNN)	Side-channel attack through RF fingerprinting	Classification accuracy > 99%	Effective detection of RF fingerprints in QKD devices, highlighting side-channel vulnerabilities	Limited to lab settings; dependency on antenna gain and APD separation	Optimize for real-world settings; assess eavesdropping distances and antenna gain
Morteza Ahmadian, 2022	DNN for State of Polarization (SOP) prediction	Environmental SOP fluctuations, high costs in polarization-encoded QKD	QBER < 0.5%, KER improvement up to 89%	Enhanced key rate and security by reducing SOP fluctuation effects	Performance drops in extreme environmental conditions; high reliance on SOP prediction	Optimize DNN architectures; expand to real-world and additional QKD protocols
Mostafa Nozari, 2024	DNN for system parameter optimization	High QBER due to underwater conditions (ISI, background noise)	QBER improvement by 2 orders of magnitude	Real-time optimization for underwater QKD; improved performance under underwater noise	Limited by parameter estimation accuracy; complex underwater conditions	Extend to multi-hop QKD; explore noise reduction strategies
Tim Johann, 2023	Long Short-Term Memory (LSTM) Neural Network	Key depletion and routing inefficiencies in QKD networks	Key store depletion reduction, latency reduction	Enhanced routing efficiency; reduced key depletion and denial-of-service risk	Simulated network basis limits generalizability to real-world QKD networks	Test on real-world networks; explore alternative ML models for higher accuracy
Hang Zhang, 2022	Autoencoder for nonlinear	Nonlinear distortions in high-speed CV-QKD,	Excess noise reduction to 10^{-3} level, improved	Effective real-time nonlinear distortion	Dependency on neural network model	Real-time implementation, adapt to other

	compensation	affecting key rates	secure key rate	compensation in CV-QKD	accuracy; generalization issues across hardware	impairments, apply to experimental setups
Bommi R.M., 2023	Deep Learning, Unsupervised Learning, Reinforcement Learning	Noise, eavesdropping, quantum attacks, and hardware imperfections in QKD systems	Key generation rate accuracy, eavesdropping detection rate	Enhanced efficiency and security in QKD through dynamic adjustment and optimization	High data requirements; vulnerability to adversarial attacks	Extend to other protocols; improve robustness in real-world conditions
Pouya Mehdizadeh, 2024	KNN, NN, and XGB	Impact of classical traffic load and spectrum usage on QKD secure key rates	High accuracy in optimal frequency prediction	Improved frequency selection for QKD and classical coexistence	Limited classical communication rate and quantum distance	Explore larger datasets and real-world applications
Brice Colombier, 2023	Random Forest for power analysis	Side-channel vulnerabilities in cryptographic systems affecting QKD	Success rate in message recovery	Demonstrated vulnerabilities in post-quantum cryptographic systems	Effectiveness depends on implementation and environmental factors	Test across broader datasets; optimize for lower computing complexity
Jiaxin Xu, 2024	Random Forest	Detection of device imperfections and eavesdropping in QKD	98% accuracy for imperfection and attack classification	High accuracy in real-time imperfection and attack detection	Potential misjudgments with 2% error rate; limited security strategy compatibility	Implement advanced strategies to reduce error rates; apply to other QKD protocols
Jing-Yang Liu, 2019	Long Short-Term Memory (LSTM) Neural Network	Phase modulation inefficiencies in QKD systems	Improved transmission efficiency (duty ratio from 50% to 83%)	Effective real-time phase modulation control for QKD systems	Requires continuous model updates and monitoring for accuracy	Apply to large-scale QKD networks; optimize LSTM for diverse conditions
Wenyuan Wang, 2019	Feedforward Neural Network	Parameter optimization inefficiencies in QKD for low-power devices	Secure key rate achievement (95-99% of optimal)	Enhanced efficiency in QKD parameter optimization	May require retraining for different conditions or protocols	Expand to additional optimization tasks, such as polarization control
Zi-Ang Ren, 2021	RF, SVM, KNN, MNB, CNN	Real-time protocol selection for secure	RF accuracy 98%, high AUC	Enabled real-time protocol selection in	Limited to studied protocols; potential	Expand to more protocols and complex QKD networks

		communication		QKD for improved security and efficiency	inaccuracies with imbalanced data	
Yiyu Mao, 2020	Artificial Neural Network (ANN)	Detection of quantum attacks in CVQKD systems	High precision and recall for attack detection accuracy	Effective real-time quantum attack detection in CVQKD	Slight reduction in secret key rate and transmission distance	Apply to additional attack types; improve model efficiency
Jia-Le Kang, 2023	Neural Networks: BPNN, RBFNN, GRNN	Inefficiency in Twin-Field QKD parameter optimization	Key rates comparable to traditional methods, faster computation	Improved secure key generation rates through neural network-based parameter optimization	May require retraining for different QKD setups	Expand model for other protocols and large-scale networks
Yuling Yi, 2021	Random Forest with data preprocessing	Signal strength and transmission probability optimization	High prediction accuracy for QKD parameters	Improved efficiency and key rate accuracy in QKD	Dependent on simulated data quality	Refine Random Forest for improved accuracy; test on diverse QKD protocols
Hua-Jian Ding, 2020	Random Forest for parameter optimization	Real-time QKD parameter optimization for large-scale networks	99% optimal key rate with reduced computation time	Enhanced QKD key rates with reduced computational demands	May vary across different QKD configurations	Extend to additional protocols and network conditions
Hong-fu Chou, 2024	Gaussian Mixture Model (GMM) and Bayes Classifier	Detection of Trojan-horse attacks and time-variant vulnerabilities in QKD networks	Improved Trojan-horse attack detection and risk-aware thresholding	Enhanced trust in QKD networks by mitigating Trojan-horse attack risks through risk-aware ML	Model effectiveness varies with quantum channel conditions; quality dependent on empirical data	Explore risk-aware reinforcement learning for real-time detection and enhance detection mechanisms in QKD networks