Table 1 Comparative Analysis of Stochastic and Machine Learning Methods

For Skin Permeability Coefficient Prediction

Method	**Euler–Maruyama Method**	**Milstein Scheme**	**Heston Model**	**Levenberg-Marquardt Method**	**Gradient Boost Regression**	**Support Vector Regression**
Type	Stochastic numerical method	Stochastic numerical method	Stochastic volatility model	Optimization algorithm	Ensemble machine learning method	Kernel-based machine learning method
Primary Purpose	Numerical approximation of stochastic differential equations (SDEs)	Numerical approximation of SDEs with improved accuracy	Modeling systems with stochastic volatility	Nonlinear least squares curve fitting and neural network training	Predictive modeling through sequential ensemble learning	Regression through optimal hyperplane fitting in high-dimensional space
Mathematical Basis	Extension of Euler method to SDEs; incorporates Wiener process	Extends Euler–Maruyama by including higher-order Itô-Taylor expansion terms	Two-dimensional SDE system coupling asset price with variance	Combination of gradient descent and Gauss-Newton methods	Sequential addition of weak learners minimizing loss function via gradient descent	Minimization of ε-insensitive loss function with regularization; kernel trick for nonlinearity
Order of Convergence	Strong order 0.5; Weak order 1.0	Strong order 1.0; Weak order 1.0	Depends on discretization scheme applied	Iterative; convergence depends on initial conditions and damping parameter	Iterative; controlled by learning rate and number of estimators	Convergence depends on kernel selection and hyperparameter tuning
Key Equation Component	Drift term + Diffusion term × Random increment	Drift term + Diffusion term × Random increment + Correction term involving diffusion derivative	Drift process + Correlated Wiener processes for price and volatility	Jacobian matrix computation; adaptive damping parameter (λ)	Negative gradient of loss function; additive combination of decision trees	Lagrangian multipliers; kernel function (RBF, linear, polynomial); slack variables
Handling of Noise	Additive Gaussian noise through Wiener increments	More accurate capture of multiplicative noise effects	Models time-varying, mean-reverting stochastic volatility	Does not inherently model stochastic noise; deterministic optimization	Robust to noise through ensemble averaging; regularization parameters	Robust to outliers through ε-insensitive tube; soft margin allows tolerance

Computational Complexity	Low; simple to implement	Moderate; requires computation of diffusion derivatives	Higher; involves solving coupled SDEs	Moderate to high; requires Jacobian computation at each iteration	Moderate to high; depends on number of trees and depth	Moderate; scales with training data size; kernel computation intensive
Key Hyperparameters	Time step size (Δt)	Time step size (Δt)	Mean reversion rate; long-term variance; volatility of volatility; correlation	Damping parameter (λ); convergence tolerance	Number of estimators; learning rate; maximum depth; minimum samples per leaf	Kernel type; regularization parameter (C); epsilon (ε); gamma (for RBF kernel)
Advantages	Simplicity; computational efficiency; easy implementation	Higher accuracy than Euler–Maruyama for same step size	Captures volatility clustering and mean reversion; realistic for financial data	Fast convergence near optimum; robust for nonlinear problems	High predictive accuracy; handles nonlinear relationships; feature importance ranking	Effective in high-dimensional spaces; robust to overfitting; handles nonlinear relationships
Limitations	Lower accuracy; may require smaller time steps	More complex implementation; requires differentiable diffusion coefficient	Parameter estimation can be challenging; computationally intensive	May converge to local minima; sensitive to initial parameter estimates	Prone to overfitting if not regularized; computationally expensive for large datasets	Sensitive to hyperparameter selection; less interpretable; slower training on large datasets
Typical Applications	Physics simulations; financial modeling; biological systems	Financial derivatives pricing; scientific simulations requiring higher precision	Options pricing; risk management; volatility forecasting	Neural network training; parameter estimation; regression analysis	Predictive analytics; ranking systems; anomaly detection; QSAR/QSPR modeling	Pattern recognition; bioinformatics; QSAR/QSPR modeling; time series forecasting
Performance in This Study	R^2 = 0.81; MSE = 0.5259	R^2 = 0.74; MSE = 0.634	R^2 = 0.72; MSE = 0.66	R^2 = 0.58; MSE = 0.94	R^2 = 0.84; MSE = 0.45	R^2 = 0.78; MSE = 0.62
Ranking by R^2 Value	2nd	4th	5th	6th	1st	3rd
Ranking by MSE Value	2nd	4th	5th	6th	1st	3rd