Scientific computing and data analytics have become the third and fourth pillars of scientific discovery. Their success is tightly linked to a rapid increase in the size and complexity of problems and datasets of interest. In this talk, I will discuss our recent efforts in the development of novel numerical algorithms for tackling these challenges. In the first part, I will present a stochastic Lanczos algorithm for estimating the spectrum of Hermitian matrix pencils. The proposed algorithm only accesses the matrices through matrix-vector products and is suitable for large-scale computations. This algorithm is one of the key ingredients in the new breed of “spectrum slicing”-type eigensolvers for electronic structure calculations. In the second part, I will present our newly developed fast structured direct solvers for kernel systems and its applications in accelerating the learning process. By exploiting intrinsic low-rank property associated with the coefficient matrix, these structured solvers could overcome the cubic solution cost and quadratic storage cost of standard dense direct solvers and provide a new framework for performing various matrix operations in linear complexity.