## GQCP::BaseOrbitalOptimizer # is converged # convergence threshold # maximum\_number\_of\_iterations # number\_of\_iterations + BaseOrbitalOptimizer() + ~BaseOrbitalOptimizer() + calculateNewRotationMatrix() + checkForConvergence() + prepareConvergenceChecking() + numberOfIterations() + optimize() GQCP::NewtonOrbitalOptimizer GQCP:: Jacobi Orbital Optimizer # hessian modifier # dim # gradient # optimal jacobi with # hessian scalar + NewtonOrbitalOptimizer() + JacobiOrbitalOptimizer() + ~NewtonOrbitalOptimizer() + ~JacobiOrbitalOptimizer() + calculateGradientMatrix() + calculatelacobiCoefficients() + calculateHessianTensor() + calculateOptimalRotation + calculateNewFullOrbitalGenerators() + prepareOrbitalDerivatives + calculateScalarFunctionChange() Calculation() + preparelacobiSpecificConvergence + calculateNewRotationMatrix() + checkForConvergence() Checking() + calculateNewRotationMatrix() + prepareConvergenceChecking() + calculateGradientVector() + checkForConvergence() + prepareConvergenceChecking() + calculateHessianMatrix() + calculateOptimalJacobiParameters() + calculateNewFreeOrbitalGenerators() + directionFromIndefiniteHessian() + comparer() + newtonStepIsWellDefined() GOCP::OCMethodNewtonOrbital Optimizer GQCP::AP1roGJacobiOrbital GQCP::ERNewtonLocalizer Optimizer # D GQCP::ERJacobiLocalizer # d + ~QCMethodNewtonOrbitalOptimizer() + AP1roGJacobiOrbitalOptimizer() + ERNewtonLocalizer() + calculateJacobiCoefficients() + calculate1DM() + AP1roGlacobiOrbitalOptimizer() + calculateGradientMatrix() + calculateOptimalRotation + calculate2DM() + calculateJacobiCoefficients() + calculateHessianTensor() + prepareDMCalculation() Angle() + calculateOptimalRotation + calculateNewFullOrbitalGenerators() + calculateGradientMatrix() + calculateScalarFunctionChange() Angle() + prepareOrbitalDerivatives + prepareJacobiSpecificConvergence + calculateHessianTensor() + calculateScalarFunctionChange() Calculation() Checking() + prepareOrbitalDerivatives + calculateGradientMatrixElement() + prepareJacobiSpecificConvergence + JacobiOrbitalOptimizer() Calculation() Checking() + calculateHessianTensorElement() + oneDM() + electronicEnergy() + twoDM() + NewtonOrbitalOptimizer() GQCP::AP1roGLagrangianNewton OrbitalOptimizer + AP1roGLagrangianNewtonOrbital Optimizer() + AP1roGLagrangianNewtonOrbital Optimizer() + prepareDMCalculation() + calculate1DM() + calculate2DM() + calculateNewFullOrbitalGenerators() + electronicEnergy() + geminalCoefficients() + multipliers()