# GQCP::BaseOrbitalOptimizer

- # is\_converged
- # convergence\_threshold
- # maximum\_number\_of\_iterations
  # number of iterations
- + BaseOrbitalOptimizer()
- + ~BaseOrbitalOptimizer()
- + calculateNewRotationMatrix()
- + checkForConvergence()
- + prepareConvergenceChecking()
- + numberOfIterations()
- + optimize()



### GQCP::NewtonOrbitalOptimizer

- # hessian modifier
- # gradient
- # gradient # hessian
  - + NewtonOrbitalOptimizer()
  - + ~NewtonOrbitalOptimizer()
  - + calculateGradientMatrix()
  - + calculateHessianTensor() + calculateNewFullOrbitalGenerators()
  - + prepareOrbitalDerivatives

## Calculation()

- + calculateNewRotationMatrix()
- + checkForConvergence()
- + prepareConvergenceChecking()
- + calculateGradientVector()
- + calculateHessianMatrix()
- + calculateNewFreeOrbitalGenerators()
- + directionFromIndefiniteHessian()
- + newtonStepIsWellDefined()



### GQCP::ERNewtonLocalizer

- + ERNewtonLocalizer()
- + calculateGradientMatrix()
- + calculateHessianTensor()
- + calculateNewFullOrbitalGenerators()
- + prepareOrbitalDerivatives

#### Calculation()

- + calculateGradientMatrixElement()
- + calculateHessianTensorElement()