# Robust Interior Point Methods and FR for Key Rate Computation in Quantum Key Distribution 

Henry Wolkowicz

Dept. Comb. and Opt., Univ. of Waterloo, Canada
(joint with: Hao Hu, Jiyoung (Haesol) Im, Jie Lin, Norbert Lütkenhaus)
Mon. April 5, 2021, 15:30 CEST At: One World Optimization Seminar


## Motivation/Outline

- find reliable, efficient numerical method for calculating key rates for quantum key distribution (QKD) protocols
- Currently: ill-posed models; i.e., we want to (minimize)
find reliable provable lower bound for the convex relative entropy: trace $\rho \log \rho-\sigma \log \rho$
$\sigma, \rho \succeq 0$ (positive semidefinite matrices), even though singular (opt. currently on boundary of SDP cone)
regulariz. using FACIAL REDUCTION, FR; on both constraints and nonlinear objective
- (I) theoretically proven upper and lower bounds with possible approximate FR; high precision
- (II) (Gauss-Newton) interior point approach on regularized problem; (originally singularity degree ONE>0)
- avoid current perturbation approach to get $\rho \succ 0$ (pos. def.)


## QKD Background (Details in References)

- Quantum key distribution, QKD: the art of distributing secret keys between two honest parties, traditionally known as Alice and Bob;
- secret key rate (number of bits of secret key obtained per exchange of quantum signal) calculation is at the core of a security proof for any QKD protocol;
- calculation is a convex minimization (lower bound) problem, s.t. constraints to detect presence of any third party (Eve eavesdropping); fundamentally: security comes from the Heisenberg uncertainty principle as eavesdropping means detectable disturbances so Alice and Bob can detect presence of Eve;
- even with a quantum computer, a secret key generated by QKD remains secure.


## (asymptotic) Key Rate Calculation

## Winick, Lütkenhaus, Coles [9]

$$
\begin{array}{ll}
p^{*}=\quad \min _{\rho} & D(\mathcal{G}(\rho) \| \mathcal{Z}(\mathcal{G}(\rho))) \\
\text { s.t. } & \Gamma(\rho)=\gamma, \quad(\text { trace } \rho=1) \\
& \rho \succeq 0 \quad(\text { density matrices })
\end{array}
$$

Here:

- $D(\delta \| \sigma)=f(\delta, \sigma)=\operatorname{trace} \delta[\log \delta-\log \sigma]$ is the quantum relative entropy;
- 「: $\mathbb{H}^{n} \rightarrow \mathbb{R}^{m}$ lin. transf., $\Gamma(\rho)=\left(\right.$ trace $\left.\Gamma_{i} \rho\right)=\left(\left\langle\Gamma_{i}, \rho\right\rangle\right)$;
- $\mathbb{H}^{n}$ linear space Hermitian matrices over $\mathbb{R} ; \gamma \in \mathbb{R}^{m}$
- $\mathcal{G}$ and $\mathcal{Z}$ are linear, completely positive maps, CP (here, sums of products $Z_{i} \rho Z_{i}^{*}$ )

$$
\begin{aligned}
& \mathrm{CP} \mathcal{G}, \mathcal{Z} ; \quad \text { e.g., } \mathcal{G}: \mathbb{H}^{n} \rightarrow \mathbb{H}^{k}, k>n, \mathcal{G}\left(\mathbb{H}_{+}^{n}\right) \subseteq \mathbb{H}_{+}^{k} \\
& \text { e.g. } \mathcal{G}(\rho)=\sum_{j=1}^{t} K_{j} \rho K_{j}^{*}, \quad \sum_{j=1}^{t} K_{j}^{*} K_{j} \preceq I .
\end{aligned}
$$

## Linear Maps $\mathcal{G}, \mathcal{Z}$

## Definition $\left(\mathcal{G}: \mathbb{H}^{n} \rightarrow \mathbb{H}^{k}\right.$ (Kraus repres.))

$$
\mathcal{G}(\rho):=\sum_{j=1}^{\ell} K_{j} \rho K_{j}^{*},
$$

$K_{j} \in \mathbb{C}^{k \times n}, \sum_{j=1}^{\ell} K_{j}^{*} K_{j} \preceq I ;$ adjoint $\mathcal{G}^{*}(\delta):=\sum_{j=1}^{\ell} K_{j}^{*} \delta K_{j} ;$
Generally $k=i * n>n, i=2,3, \ldots$; and so typically $\mathcal{G}(\rho)$ rank deficient $\forall \rho \succ 0$ (positive definite)

Definition (self-adjoint (projection) $\mathcal{Z}: \mathbb{H}^{k} \rightarrow \mathbb{H}^{k}$ )

$$
\mathcal{Z}(\delta):=\sum_{j=1}^{N} Z_{j} \delta Z_{j}
$$

$Z_{j}=Z_{j}^{2}=Z_{j}^{*} \in \mathbb{H}_{+}^{k}$ and $\sum_{j=1}^{N} Z_{j}=I_{k}$

## Properties of QKD Problem

## Lemma

The linear map $\mathcal{Z}$ is an orthogonal projection on $\mathbb{H}^{k}$ and trace $(\delta) \leq 1, \delta \succ 0$ implies:

$$
\operatorname{trace}(\delta \log \mathcal{Z}(\delta))=\operatorname{trace}(\mathcal{Z}(\delta) \log \mathcal{Z}(\delta))
$$

$\mathcal{G}, \mathcal{Z} \circ \mathcal{G}$ May not Preserve Positive Definiteness

$$
\begin{array}{lll}
p^{*}= & \min _{\rho} & D(\mathcal{G}(\rho) \| \mathcal{Z}(\mathcal{G}(\rho))) \\
\text { s.t. } & \Gamma(\rho)=\gamma, \\
& \rho \succeq 0 \quad \text { (density matrices) }
\end{array}
$$

## Known Properties

$$
\min _{\rho, \sigma, \delta} \operatorname{trace}(\delta(\log \delta))-\operatorname{trace}(\sigma(\log \sigma))
$$

quantum relative entropy $D$ is finite under range condition; jointly convex in both $\delta$ and $\sigma$

## Equivalent Formulation

Ready for FR, Facial Reduction (Regularization)

$$
\begin{array}{lll}
p^{*}=\quad \min _{\rho, \sigma, \delta} & \operatorname{trace}(\delta(\log \delta))-\operatorname{trace}(\sigma(\log \sigma)) \\
\text { s.t. } & \Gamma(\rho)=\gamma \\
& \sigma=\mathcal{Z}(\delta) \\
& \delta=\mathcal{G}(\rho) \\
& \rho, \sigma, \delta \succeq 0
\end{array}
$$

## Our Goal: Final Asymptotic Key Rate

obtained by getting a reliable lower bound of this problem (and then removing the cost of error correction, a constant).

## Facial Reduction, FR, Borwein-W. [3], Preliminaries

## Slater Constraint Qualification, Strict Feasibility, Stability

Slater: $\exists \hat{\rho} \succ 0:\lceil\hat{\rho}=\gamma$

## Strong Duality, Stability

Slater is sufficient for strong duality;
equivalent to numerical stability under RHS perturbations; Slater fails in surprisingly many applications

## Advantages of FR

FR can be used to obtain strict feasibility and regularize the problem, and often simultaneously simplify the problem.

## current applications: e.g.

hard discrete opt.; (distance geometry); EDM and low rank matrix completion etc ... (recent survey Drusvyatskiy-W. [5])

## Facial Reduction, FR, Preliminaries cont...

convex cone: $K: \lambda K \subseteq K, \forall \lambda \geq 0, K+K \subset K$, dual cone: $S^{*}=\{\phi \in \mathbb{H}:\langle\phi, s\rangle \geq 0, \forall s \in S\}$. convex cone $F$ is a face of a convex cone $K, F \unlhd K$, if

$$
x, y \in K, x+y \in F \Longrightarrow x, y \in F
$$

Faces of the positive semidefinite cone are characterized by the range or nullspace of any element in the relative interior:

## Lemma

Let $F$ a convex subset of $\mathbb{H}_{+}^{n}$ with $X \in$ ri $F$ with orthogonal spectral decomposition $X=\left[\begin{array}{ll}P & Q\end{array}\right]\left[\begin{array}{ll}D & 0 \\ 0 & 0\end{array}\right]\left[\begin{array}{ll}P & Q\end{array}\right]^{*}$, with $D \in \mathbb{H}_{++}^{r}$. Then TFAE:
(i) $F \unlhd \mathbb{H}_{+}^{n}$;
(ii) $F=\left\{Y \in \mathbb{H}_{+}^{n}:\right.$ range $\left.(Y) \subset \operatorname{range}(X)\right\}$

$$
=\left\{Y \in \mathbb{H}_{+}^{n}: \operatorname{null}(Y) \supset \operatorname{null}(X)\right\} ;
$$

(iii) $F=P \mathbb{H}_{+}^{r} P^{*}$; (iv) $F=\mathbb{H}_{+}^{n} \cap\left(Q Q^{*}\right)^{\perp}$ (exposing $Q Q^{*}$ )

## Facial Reduction via Theorem of Alternative

## Lemma (theorem of the alternative)

For the feasible constraint system, exactly one of the following statements holds:
(1) there exists $\rho \succ 0$ such that $\Gamma(\rho)=\gamma$ (Slater);
(2) there exists $y$ (and exposing vector $Z$ ) such that

$$
0 \neq Z=\Gamma^{*}(y) \succeq 0,\langle\gamma, y\rangle=0
$$

The matrix $Z=\Gamma^{*} y$ above is an exposing vector for the feasible set.

## Definition (minimal face)

$K$ a closed convex cone; $S \subseteq K$ a convex set; then face $(S) \unlhd K$ is the minimal face, the intersection of all faces of $K$ that contain $S$.

## First (Partial) FR Step on $S_{R}$ (Analytical/Accurate)

## affine manifold constraint is divided into two sets

observable, reduced density operator constraint sets, $S_{O} \cap S_{R}$; with Kronecker product, $\otimes$

$$
\begin{aligned}
& S_{O}=\left\{\rho \succeq 0:\left\langle P_{s}^{A} \otimes P_{t}^{B}, \rho\right\rangle=p_{s t}, \forall s, t\right\}, \\
S_{R} & =\left\{\rho \succeq 0: \operatorname{trace}_{B}(\rho)=\rho_{A}\right\} \quad \text { (partial trace) } \\
& =\left\{\rho \succeq 0:\left\langle\left.\Theta_{j} \otimes\right|_{B}, \rho\right\rangle=\theta_{j}, \forall j=1, \ldots, m_{R}\right\},
\end{aligned}
$$

## where

data $\theta_{j}=\left\langle\Theta_{j}, \rho_{A}\right\rangle$; and $\rho_{A} \in \mathbb{H}_{+}^{n_{A}}$ often singular $\left\{\Theta_{j}\right\}$ orthonormal basis system $A$.

Let range $P=$ range $\rho_{A} \subsetneq \mathbb{H}^{n_{A}}, P^{*} P=I_{r}$, and let $V=P \otimes I_{B}$. Then $\mathrm{FR}: \rho \in S_{R} \Longrightarrow \rho=V R V^{*}$, for some $R \in \mathbb{H}_{+}^{r \cdot n_{B}}$

## FR on the Objective Function

Lemma (useful equivalent form for entropy function)
Let $Y=V R V^{*} \in \mathbb{H}_{+}, R \succ 0$ be the compact spectral decomposition of $Y$ with $V^{*} V=I$. Then

$$
\operatorname{trace}(Y \log Y)=\operatorname{trace}(R \log R)
$$

## Proof.

We obtain a unitary matrix $U=\left[\begin{array}{ll}V & P\end{array}\right]$ by completing the basis. Then $Y=U D U^{*}$, where $D=\operatorname{BlkDiag}(R, 0)$. We conclude, with $0 \cdot \log 0=0$, that trace $Y \log Y=\operatorname{trace} D \log D=$ trace $R \log R$.

## Exposing Vectors Analytically; Spectral Decomposition

We use the following simple result to obtain the exposing vectors of the minimal face in the problem analytically, i.e., we find the matrices $V$ with orthonormal columns.

## Lemma (analytic FR)

Let $\mathcal{C} \subseteq \mathbb{H}_{+}^{n}$ be a given closed convex set with nonempty interior. Let $Q_{i} \in \mathbb{H}^{k \times n}, i=1, \ldots, t$, be given matrices. Define the linear map $\mathcal{A}: \mathbb{H}^{n} \rightarrow \mathbb{H}^{k}$ and matrix $V$ by

$$
\mathcal{A}(X)=\sum_{i}^{t} Q_{i} X Q_{i}^{*}, \quad \text { range }(V)=\operatorname{range}\left(\sum_{i=1}^{t} Q_{i} Q_{i}^{*}\right)
$$

Then the minimal face,

$$
\operatorname{face}(\mathcal{A}(\mathcal{C}))=V \mathbb{H}_{+}^{r} V^{*}
$$

## Obtain the Minimal Faces, $V \mathbb{H}_{+} V^{*}$

$$
\begin{aligned}
& \rho=V_{\rho} R_{\rho} V_{\rho}^{*} \in \mathbb{H}_{+}^{n}, \quad R_{\rho} \in \mathbb{H}_{+}^{n_{\rho}} \\
& \delta=V_{\delta} R_{\delta} V_{\delta}^{*} \in \mathbb{H}_{+}^{k}, \quad R_{\delta} \in \mathbb{H}_{+}^{\kappa_{\delta}} \\
& \sigma=V_{\sigma} R_{\sigma} V_{\sigma}^{*} \in \mathbb{H}_{+}^{k}, \quad R_{\sigma} \in \mathbb{H}_{+}^{k_{\sigma}}
\end{aligned}
$$

Define the linear maps

$$
\begin{array}{lll}
\Gamma_{V}: \mathbb{H}_{n_{\rho}}^{n_{\rho}} \rightarrow \mathbb{R}^{m} & \text { by } \quad \Gamma_{V}\left(R_{\rho}\right)=\Gamma\left(V_{\rho} R_{\rho} V_{\rho}^{*}\right), \\
\mathcal{G}_{V}: \mathbb{H}_{R_{p}} \rightarrow \mathbb{H}_{+}^{k} & \text { by } & \mathcal{G}_{V}\left(R_{\rho}\right)=\mathcal{G}\left(V_{\rho} R_{\rho} V_{\rho}^{*}\right), \\
\mathcal{Z}_{V}: \mathbb{H}_{+}^{k_{k}} \rightarrow \mathbb{H}_{+}^{k} & \text { by } & \mathcal{Z}_{V}\left(R_{\delta}\right)=\mathcal{Z}\left(V_{\delta} R_{\delta} V_{\delta}^{*}\right) .
\end{array}
$$

## Substitute with Linear Mapping $\mathcal{V}_{\delta}(\cdot):=V_{\delta} \cdot V_{\delta}^{*}$

## Equivalent Formulation

$$
\min \quad \operatorname{trace}\left(R_{\delta} \log \left(R_{\delta}\right)\right)-\operatorname{trace}\left(R_{\sigma} \log \left(R_{\sigma}\right)\right)
$$

subject to: $\quad \Gamma_{V}\left(R_{\rho}\right)=\gamma$

$$
\begin{aligned}
& \mathcal{V}_{\sigma}\left(R_{\sigma}\right)-\mathcal{Z}_{V}\left(R_{\delta}\right)=0 \\
& \mathcal{V}_{\delta}\left(R_{\delta}\right)-\mathcal{G}_{V}\left(R_{\rho}\right)=0 \\
& R_{\rho}, R_{\sigma}, R_{\delta} \succeq 0 .
\end{aligned}
$$

## After Rotation and Substitution; final model (QKD)

$$
\begin{aligned}
p^{*}=\quad \min \quad f(\rho)= & \operatorname{trace}(\widehat{\mathcal{G}}(\rho)(\log \widehat{\mathcal{G}}(\rho))) \\
& -\operatorname{trace}(\widehat{\mathcal{Z}}(\rho) \log \widehat{\mathcal{Z}}(\rho))
\end{aligned}
$$

subject to: $\Gamma_{V}(\rho)=\gamma_{V}$

$$
\rho \in \mathbb{H}_{+}^{n_{\rho}},
$$

Slater holds; smaller regularized problem; positive definiteness preserved in obj. fn

## Derivatives

## Theorem (Derivatives of regularized objective)

Let $\rho \succ 0$. The gradient of $f$ is

$$
\nabla f(\rho)=\widehat{\mathcal{G}}^{*}(\log [\widehat{\mathcal{G}}(\rho)])+\widehat{\mathcal{G}}^{*}(I)-\widehat{\mathcal{Z}}^{*}(\log [\widehat{\mathcal{Z}}(\rho)])+\widehat{\mathcal{Z}}^{*}(I) \text {. }
$$

The Hessian in direction $\Delta \rho$ is (1st order info)

$$
\begin{aligned}
\nabla^{2} f(\rho)(\Delta \rho)= & \hat{\mathcal{G}}^{*}\left(\log ^{\prime}[\hat{\mathcal{G}}(\rho)](\hat{\mathcal{G}}(\Delta \rho))-\right. \\
& \hat{\mathcal{Z}}^{*}\left(\log ^{\prime}[\hat{\mathcal{Z}}(\rho)](\hat{\mathcal{Z}}(\Delta \rho))\right.
\end{aligned}
$$

## Theorem (subdifferential)

Let $\left\{\rho_{i}\right\}_{i} \subseteq \mathbb{S}_{++}^{n_{p}}$ with $\rho_{i} \rightarrow \bar{\rho}$. If we have the convergence $\lim _{i} \nabla f\left(\rho_{i}\right)=\phi$, then

$$
\phi \in \partial f(\bar{\rho}) .
$$

## Part II: Opt. Cond.; Bounds; GN Int. Pt. Method

- Duality, and primal-dual optimality conditions with null-space representation
- Derive a Gauss-Newton search direction for the nonlinear SDP (with exact primal and dual feasibility possible)
- derive provable lower and upper bounds
- Empirics

Facially Reduced (Regularized) Nonlinear SDP

$$
\begin{array}{ll}
p^{*}=\quad \min _{\text {subject to: }}: & f(\rho) \quad \text { (regularized relative entropy) } \\
& \Gamma \vee(\rho)=\gamma_{V} \quad \text { (FR constraints) } \\
& \rho \in \mathbb{H}_{+}^{n_{\rho}} \quad \text { (smaller SDP constr.) }
\end{array}
$$

## Duality/Optimality

## Theorem (Basic Duality/Opt)

(1) Lagrangian $L(\rho, y)=f(\rho)+\left\langle y, \Gamma_{V} \rho-\gamma v\right\rangle, y \in \mathbb{R}^{m_{v}}$.
(2) Strong Duality

$$
\begin{aligned}
p^{*} & =\max _{y} \min _{\rho \succeq 0} L(\rho, y) \\
& =d^{*}=\max _{Z \succeq 0, y}\left(\min _{\rho}(L(\rho, y)-\langle Z, \rho\rangle)\right)
\end{aligned}
$$

and $d^{*}$ is attained for some $(y, Z) \in \mathbb{R}^{m_{v}} \times \mathbb{H}_{+}^{n_{\rho}}$.
(3) p-d pair $(\rho,(y, Z))$, with $\partial f(\rho) \neq \emptyset$, is optimal iff

$$
\begin{array}{lll}
0 & \in \partial f(\rho)+\Gamma_{v^{*}} y-Z & \text { (dual feasibility) } \\
0=\Gamma_{v} \rho-\gamma v & \text { (linear primal feasibility) } \\
0=\langle\rho, Z\rangle & \text { (complementary slackness) } \\
0 \preceq \rho, Z & \text { (SDP primal feasibility). }
\end{array}
$$

Moreover, $\Gamma_{V}^{*} y \succeq 0,\left\langle y, \gamma_{V}\right\rangle<0$, for some $y$, implies infeas.

## Nullspace Representation/Residuals

## Definition (nullspace representation)

$\hat{\rho} \in \mathbb{H}^{n_{\rho}}$ feasible point for $\Gamma_{V}(\cdot)=\gamma_{v}$.
$\mathcal{N}^{*}: \mathbb{R}^{n_{\rho}^{2}-m_{v}} \rightarrow \mathbb{H}^{n_{\rho}}$ injective linear map in adjoint form so that we have the nullspace representation for the residual:

$$
F_{\mu}^{p}=\Gamma_{v} \rho-\gamma_{v} \Longleftrightarrow F_{\mu}^{p}=\mathcal{N}^{*}(v)+\hat{\rho}-\rho, \text { for some } v .
$$

## Perturbed Optimality Conditions/Residuals

(i) dual feas.; (ii) primal feas.; (iii) perturbed compl. slack.

$$
F_{\mu}(\rho, v, y, Z)=\left[\begin{array}{c}
F_{\mu}^{d} \\
F_{\mu}^{p} \\
F_{\mu}^{c}
\end{array}\right]=\left[\begin{array}{c}
\nabla_{\rho} f(\rho)+\Gamma_{v^{*}} y-Z \\
\mathcal{N}^{*} v+\hat{\rho}-\rho \\
Z \rho-\mu l
\end{array}\right]=0, \quad \rho, Z \succ 0 .
$$

EXACT p -d feas if updated as: $\rho \leftarrow \Delta v ; Z \leftarrow \Delta \rho, \Delta y$; after a steplength $=1$ is taken, exact p.f. is maintained. exact dual feas. for $Z$ is key for lower bound

## Projected Gauss-Newton P-D I-P Method

Linearized System for GN Direction; OVERDETERMINED

$$
F_{\mu}^{\prime} d_{G N}=\left[\begin{array}{c}
\nabla^{2} f(\rho) \Delta \rho+\Gamma v^{*} \Delta y-\Delta Z \\
\mathcal{N}^{*}(\Delta v)-\Delta \rho \\
Z \Delta \rho+\Delta Z \rho
\end{array}\right] \approx-F_{\mu}
$$

From First Block (for backsubstitution)

$$
\begin{aligned}
\Delta Z & =F_{\mu}^{d}+\nabla^{2} f(\rho) \Delta \rho+\Gamma v^{*} \Delta y \\
& =F_{\mu}^{d}+\nabla^{2} f(\rho)\left(F_{\mu}^{p}+\mathcal{N}^{*}(\Delta v)\right)+\Gamma v^{*} \Delta y
\end{aligned}
$$

From Second Block (for backsubstitution)

$$
\Delta \rho=F_{\mu}^{p}+\mathcal{N}^{*}(\Delta v)
$$

Now substitute $\Delta Z, \Delta \rho$ into third block.

## Projected GN direction

$d_{G N}=\left(\begin{array}{ll}\Delta v & \Delta y\end{array}\right) \quad$ (backsubst. for $\left.\Delta \rho, \Delta Z\right)$
found from the least squares solution of (OVERDETERMINED)

$$
\begin{aligned}
& {\left[Z \mathcal{N}^{*}(\Delta v)+\nabla^{2} f(\rho) \mathcal{N}^{*}(\Delta v) \rho\right]+\left[\Gamma v^{*} \Delta y \rho\right]} \\
& =-F_{\mu}^{c}-Z F_{\mu}^{p}-\left(F_{\mu}^{d}+\nabla^{2} f(\rho) F_{\mu}^{p}\right) \rho
\end{aligned}
$$

(Uses Hessian acting on a vector: $\nabla^{2} f(\rho): \mathbb{H} \rightarrow \mathbb{H}$ )
Initialize: $\hat{\rho} \succ 0, \mu \in \mathbb{R}_{++}, \eta \in(0,1)$
WHILE: stopping criteria is not met
solve for $(\Delta v, \Delta y)$
$\Delta \rho=F_{\mu}^{p}+\mathcal{N}^{*}(\Delta v)$
$\Delta Z=F_{\mu}^{d}+\nabla^{2} f(\rho)\left(F_{\mu}^{p}+\mathcal{N}^{*}(\Delta v)\right)+\Gamma v^{*} \Delta y$
choose steplength $\alpha$
$(\rho, \boldsymbol{y}, \boldsymbol{Z}) \leftarrow(\rho, \boldsymbol{y}, \boldsymbol{Z})+\alpha(\Delta \rho, \Delta \boldsymbol{y}, \Delta \boldsymbol{Z})$
$\mu=\operatorname{trace}(\rho Z) / n ; \mu \leftarrow \eta \mu$
ENDWHILE

## Implementation Details

## Sparse Nullspace Representation

We use a matrix representation $M$ for $\Gamma$ and a row and column permutation to get a well-conditioned near triangular basis matrix $B$. nullspace representation:

$$
\hat{r}=H \operatorname{vec} \hat{\rho} ; \Gamma \vee \hat{\rho}=M \hat{r}(c p)=\gamma v, M=\left[\begin{array}{ll}
B & E
\end{array}\right], N^{*}=\left[\begin{array}{c}
B^{-1} E \\
-I
\end{array}\right]
$$

## Optimal Diagonal Preconditioning, [4]

$d_{i}=\left\|F_{\mu}^{c \prime}\left(e_{i}\right)\right\|$, for unit vectors $e_{i}$; column precondition using

$$
F_{\mu}^{c \prime} \leftarrow F_{\mu}^{c \prime} \operatorname{Diag}(d)^{-1}
$$

MATLAB: $d_{G N}=\left(\left(F_{\mu}^{c \prime} / \operatorname{Diag}(d)\right) \backslash R H S\right) . / d$
Performed exceptionally well; problems are VERY
ill-conditioned.

## Upper Bounds

## Evaluate $f$ at Feasible $\rho$; Iterative Refinement if Needed

if approximate linear feasibility $\Gamma_{V} \hat{\rho} \approx \gamma_{V}$, we apply iterative refinement by finding the projection Let $\hat{\rho} \succ 0, F_{\mu}^{p}=\Gamma_{V} \hat{\rho}-\gamma_{V}$. Then

$$
\rho=\hat{\rho}-\Gamma_{V}{ }^{\dagger} F_{\mu}^{p}=\operatorname{argmin}_{\rho}\left\{\frac{1}{2}\|\rho-\hat{\rho}\|^{2}: \Gamma_{V} \rho=\gamma_{V}\right\},
$$

where we denote $\Gamma_{V}{ }^{\dagger}$, generalized inverse. If $\rho \succeq 0$, then $p^{*} \leq f(\rho)$.

## EXACT Primal Feasibility

In our tests we take a Newton step quite early, and maintain exact primal feasibility (no roundoff error buildup) for the further iterations.

## Lower Bound from Weak Duality

## $\rho \succ 0, Z \succ 0$ in Interior Point Algorithm

The gradients exist at $\rho \succ 0$; we can verify dual feasibility.

## Corollary (Lower Bound for FR problem from EXACT Dual Feas.)

$\hat{\rho}, \hat{y}$ primal-dual iterate; $\hat{\rho} \succ 0$. Set $\bar{Z}=\nabla f(\hat{\rho})+\Gamma v^{*} \hat{y}$.
If $\bar{Z} \succeq 0$, then lower bound is:

$$
p^{*} \geq f(\hat{\rho})+\left\langle\hat{y}, \Gamma_{V} \hat{\rho}-\gamma_{v}\right\rangle-\langle\hat{\rho}, \bar{Z}\rangle .
$$

## Proof.

Consider the dual problem $d^{*}=\max _{y, Z \succeq 0} \min _{\rho \in \mathbb{H}^{n_{\rho}}} L(\rho, y)-\langle Z, \rho\rangle$. Dual feasibility implies:
$\bar{Z} \succeq 0, \nabla f(\hat{\rho})+\Gamma v^{*} \hat{y}-\bar{Z}=0 \Longrightarrow \hat{\rho} \in \operatorname{argmin}_{\rho} L(\rho, \hat{y})-\langle\bar{Z}, \rho\rangle$.
Result follows from weak duality.

## Numerics; GN vs FW with/without FR

| Problem Data |  | Gauss-Newton |  | FW (FR) |  | FW (no FR) |  | cvxquad (FR) |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| protocol | size | gap | time | gap | time | gap | time | gap | time |
| ebBB84 | $(4,16)$ | $6.0 \mathrm{e}-13$ | 0.4 | 1.0e-04 | 86.9 | 1.2e-04 | 93.9 | 5.5e-01 | 194 |
| ebBB84 | $(4,16)$ | 1.2e-12 | 0.3 | 1.7e-04 | 96.8 | 1.3e-04 | 110.5 | $5.4 \mathrm{e}-01$ | 1938 |
| ebBB84 | $(4,16)$ | 1.1e-12 | 0.2 | 1.6e-04 | 86.5 | 2.2e-04 | 112.0 | $5.7 \mathrm{e}-01$ | 1979 |
| ebBB84 | $(4,16)$ | $4.2 \mathrm{e}-13$ | 0.2 | $2.2 \mathrm{e}-04$ | 88.6 | 2.2e-04 | 111.9 | 6.3e-01 | 523 |
| pmBB84 | $(8,32)$ | $5.5 \mathrm{e}-13$ | 0.2 | $3.1 \mathrm{e}-05$ | 1.3 | $6.5 \mathrm{e}-04$ | 1.6 | 5.3e-01 | 158 |
| pmBB84 | $(8,32)$ | 6.1e-13 | 0.2 | 1.6e-04 | 1.1 | 3.8e-04 | 93.0 | 5.2e-01 | 207 |
| pmBB84 | $(8,32)$ | 6.3e-13 | 0.2 | 5.5e-05 | 1.1 | $3.0 \mathrm{e}-04$ | 112.3 | $5.6 \mathrm{e}-01$ | 299 |
| pmBB84 | $(8,32)$ | 1.3e-12 | 0.2 | 2.6e-04 | 1.1 | 1.3e-03 | 87.0 | $5.9 \mathrm{e}-01$ | 188 |
| mdiBB84 | $(48,96)$ | $7.9 \mathrm{e}-13$ | 0.9 | $9.6 \mathrm{e}-05$ | 1.6 | $5.4 \mathrm{e}-04$ | 120.9 | $1.8 \mathrm{e}-01$ | 570 |
| mdiBB84 | $(48,96)$ | $1.4 \mathrm{e}-12$ | 0.7 | $5.5 \mathrm{e}-05$ | 101.2 | $6.6 \mathrm{e}-04$ | 119.7 | $2.4 \mathrm{e}-01$ | 585 |
| mdiBB84 | $(48,96)$ | $5.7 \mathrm{e}-13$ | 0.9 | $1.5 \mathrm{e}-04$ | 101.9 | $1.7 \mathrm{e}-03$ | 439.3 | $3.1 \mathrm{e}-01$ | 584 |
| mdiBB84 | $(48,96)$ | 9.2e-13 | 0.8 | $1.8 \mathrm{e}-04$ | 100.0 | $2.2 \mathrm{e}-03$ | 441.3 | $3.7 \mathrm{e}-01$ | 558 |

Table: Numerical Report: Gauss-Newton, Frank-Wolfe (FW), cvxquad

- GN performs significantly better for both accuracy and running time
- only three protocols (each with four different parameter settings);
that is all that cvxquad could handle;
- FW is significantly improved by using our new FR


## Larger Numerics; cvxquad Failed

| Problem Data |  | Gauss-Newton |  | FW (FR) |  | FW (no FR) |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| protocol | size | gap | time | gap | time | gap | time |
| TFQKD | $(12,24)$ | $5.9 \mathrm{e}-13$ | 1.1 | $2.6 \mathrm{e}-09$ | 1.9 | $1.6 \mathrm{e}-03$ | 364.1 |
| TFQKD | $(12,24)$ | $1.2 \mathrm{e}-12$ | 0.8 | $3.8 \mathrm{e}-09$ | 1.5 | $5.6 \mathrm{e}-04$ | 369.1 |
| TFQKD | $(12,24)$ | $3.2 \mathrm{e}-13$ | 0.8 | $4.0 \mathrm{e}-09$ | 1.3 | $1.7 \mathrm{e}-04$ | 4.1 |
| DMCV | $(44,176)$ | $2.7 \mathrm{e}-09$ | 1326.1 | $2.4 \mathrm{e}-06$ | 2808.4 | $3.4 \mathrm{e}-06$ | 4933.9 |
| DMCV | $(44,176)$ | $2.7 \mathrm{e}-09$ | 1377.4 | $1.3 \mathrm{e}-06$ | 974.2 | $2.5 \mathrm{e}-06$ | 1281.2 |
| DMCV | $(48,192)$ | $3.1 \mathrm{e}-09$ | 1807.1 | $2.7 \mathrm{e}-06$ | 3167.4 | $5.1 \mathrm{e}-06$ | 5407.5 |
| DMCV | $(48,192)$ | $3.2 \mathrm{e}-09$ | 2110.6 | $2.6 \mathrm{e}-06$ | 979.8 | $2.0 \mathrm{e}-06$ | 1756.3 |
| dprBB84 | $(12,48)$ | $4.9 \mathrm{e}-13$ | 1.3 | $3.8 \mathrm{e}-06$ | 88.0 | $9.4 \mathrm{e}-05$ | 123.0 |
| dprBB84 | $(24,96)$ | $1.0 \mathrm{e}-12$ | 12.1 | $6.2 \mathrm{e}-06$ | 15.9 | $3.6 \mathrm{e}-06$ | 31.1 |
| dprBB84 | $(36,144)$ | $5.0 \mathrm{e}-13$ | 69.3 | $6.5 \mathrm{e}-04$ | 8.8 | $2.1 \mathrm{e}-02$ | 30.1 |
| dprBB84 | $(48,192)$ | $1.1 \mathrm{e}-12$ | 325.5 | $4.4 \mathrm{e}-05$ | 17.1 | $9.8 \mathrm{e}-04$ | 181.9 |

Table: Numerical Report: Gauss-Newton, Frank-Wolfe (FW)

- GN performs significantly better again
- FW does significantly better with our new FR again


## GN is Exactly Analytical (Protocol mdiBB84)



The • are the lower bounds from GN; they coincide exactly with the analytical values on the curves.
This meets with the empirical evidence of gaps $\approx 10^{-12}$

## Conclusion

- regularized the key rate calculation using FACIAL REDUCTION on both constraints and nonlinear (relative entropy) objective function over the Hermitians (complex);
- provided theoretically proven upper and lower bounds with high precision
- derived robust (Gauss-Newton) interior point approach on regularized problem
- avoids current perturbation approach to get $\rho \succ 0$;
- avoids roundoff error from backsubstitution steps;
- attains exact primal feasibility during iterations
- uses exact dual feasibility steps to improve on lower bounds


## References I



Borwein, J., and Wolkowicz, H.
Characterization of optimality for the abstract convex program with finite-dimensional range.
J. Austral. Math. Soc. Ser. A 30, 4 (1980/81), 390-411.Borwein, J., and Wolkowicz, H.
Facial reduction for a cone-convex programming problem.
J. Austral. Math. Soc. Ser. A 30, 3 (1980/81), 369-380.

Borwein, J., and Wolkowicz, H.
Regularizing the abstract convex program.
J. Math. Anal. Appl. 83, 2 (1981), 495-530.


Dennis Jr., J., and Wolkowicz, H.
Sizing and least-change secant methods.
SIAM J. Numer. Anal. 30, 5 (1993), 1291-1314.


Drusvyatskiy, D., and Wolkowicz, H.
The many faces of degeneracy in conic optimization.
Foundations and Trends ${ }^{\circledR}$ (in Optimization 3, 2 (2017), 77-170.
.
Faybusovich, L., and Zhou, C.
Long-step path-following algorithm in quantum information theory: Some numerical aspects and applications, 2020.

## References II



George, I., Lin, J., and Lütkenhaus, N.
Numerical calculations of the finite key rate for general quantum key distribution protocols.
Physical Review Research 3 (2021), 013274.
Lin, J., Upadhyaya, T., and Lütkenhaus, N.
Asymptotic security analysis of discrete-modulated continuous-variable quantum key distribution.
Phys. Rev. X 9 (2019), 041064.
Winick, A., Lütkenhaus, N., and Coles, P.
Reliable numerical key rates for quantum key distribution.
Quantum 2 (Jul 2018), 77.

## Thanks for your attention!

# Robust Interior Point Methods and FR for Key Rate Computation in Quantum Key Distribution 

Henry Wolkowicz

Dept. Comb. and Opt., Univ. of Waterloo, Canada
(joint with: Hao Hu, Jiyoung (Haesol) Im, Jie Lin, Norbert Lütkenhaus)
Mon. April 5, 2021, 15:30 CEST At: One World Optimization Seminar


