Duality Bounds Computation Notes

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1 Introduction

These are notes on the details of the numerical implementation of photonic duality bounds.

2 The Lagrangian

$$\mathcal{L}(\lambda, T) = \begin{bmatrix} \langle T| & \langle S| \end{bmatrix} \begin{bmatrix} -Z^{TT}(\lambda) & Z^{TS}(\lambda) \\ Z^{ST}(\lambda) & \mathbf{0} \end{bmatrix} \begin{bmatrix} |T\rangle \\ |S\rangle \end{bmatrix} \tag{1}$$

Since the constraints are all real (taking the real and imaginary parts of complex constraints), $Z^{TS} = Z^{ST\dagger}$. To evaluate the dual function

$$\mathcal{G}(\lambda) = \max_{|T\rangle} \mathcal{L}(\lambda, T) \tag{2}$$

We find the stationary point $|T^*\rangle$ of $\mathcal{L}$ by solving the relation (see references on Wirtinger calculus)

$$\frac{\partial \mathcal{L}}{\partial \langle T^*|} = 0 \tag{3}$$

which leads to the linear system

$$Z^{TT} |T^*\rangle = Z^{TS} |S\rangle \tag{4}$$

in order for the dual to be finite, Z^{TT} must be positive definite, so this linear system is invertible, leading to

$$|T^*\rangle = Z^{TT-1} Z^{TS} |S\rangle \tag{5}$$

$$\mathcal{G}(\lambda) = \langle S| Z^{ST} Z^{TT-1} Z^{TS} |S\rangle \tag{6}$$

It is left as an exercise for the reader to show that

$$\frac{\partial \mathcal{G}}{\partial \lambda} = 2\,\mathrm{Re}\left\{ \langle T^*| \frac{\partial Z^{TS}}{\partial \lambda} |S\rangle \right\} - \langle T^*| \frac{\partial Z^{TT}}{\partial \lambda} |T^*\rangle \tag{7}$$

3 Objective and Constraints

As a concrete example, consider limits on the scattered power from an incident field $|S\rangle$, formulated as the following QCQP

$$\begin{aligned} \underset{T}{\text{maximize}} \quad & \mathrm{Im}\,\langle S|T\rangle - \frac{\mathrm{Im}\,\chi}{|\chi|^2} \langle T|T\rangle && \text{(8a)} \\ \text{subject to} \quad & \mathrm{Re}\{\langle S| \mathbb{P}_j |T\rangle\} - \langle T| \mathrm{Sym}(\mathbb{U}\mathbb{P}_j) |T\rangle && \text{(8b)} \\ & \mathrm{Im}\{\langle S| \mathbb{P}_j |T\rangle\} - \langle T| \mathrm{Asym}(\mathbb{U}\mathbb{P}_j) |T\rangle && \text{(8c)} \end{aligned}$$

where $\mathbb{U} = \chi^{-1\dagger} - \mathbb{G}^\dagger$. Now, assign the multiplier λ_{2j} to the real $\mathbb{P}_j$ constraint and λ_{2j+1} to the imaginary $\mathbb{P}_j$ constraint. The sub-blocks of the Lagrangian take the form

$$Z^{TT}(\lambda) = \mathbb{O}_{quad} + \sum_j \big(\lambda_{2j}\mathrm{Sym}(\mathbb{U}\mathbb{P}_j) + \lambda_{2j+1}\mathrm{Asym}(\mathbb{U}\mathbb{P}_j)\big) \tag{9a}$$

$$Z^{TS}(\lambda)\,|S\rangle = \mathbb{O}_{lin} + \sum_j \big(\frac{\lambda_{2j}}{2}\,|S\rangle + \frac{i\lambda_{2j+1}}{2}\,|S\rangle\,\big) \tag{9b}$$

$$\mathbb{O}_{quad} = \frac{\mathrm{Im}\,\chi}{|\chi|^2}\mathbb{I} \tag{9c}$$

$$\mathbb{O}_{lin} = \frac{i}{2}\,|S\rangle \tag{9d}$$

where $\emptyset_{lin}$ and $\emptyset_{quad}$ are the linear and quadratic parts of the objective.

4 Optimization of the Dual Function

Use equation (7) to evaluate gradient of dual function with respect to the Lagrangian multipliers λ and use first-order optimization methods. If desired, can also efficiently compute Hessian of dual function and use second-order optimization methods.

4.1 Fake Sources

When minimizing the dual (2) we must always enforce the domain of duality constraint $Z^{TT} \succ 0$. Consider the eigenvector decomposition of Z^{TT}

$$Z^{TT} = \sum_k q_k\,|v_k\rangle\,\langle v_k| \qquad q_k \in \mathbb{R} \qquad q_1 \le \cdots \le q_n$$
$$Z^{TT-1} = \sum_k q_k^{-1}\,|v_k\rangle\,\langle v_k|$$

When we approach the duality boundary where Z^{TT} becomes singular, $q_1 \to 0$. The form of the dual in (6) suggests that as we approach the duality boundary where Z^{TT} becomes singular, the dual $\mathcal{G}(\lambda)$ should diverge if $\langle v_1|\,Z^{TS}\,|S\rangle \neq 0$. In this favorable scenario, the gradient of the dual will push the optimization algorithm away from the duality boundary.
However in certain cases $\langle v_1|\,Z^{TS}\,|S\rangle \to 0$ as we approach the duality boundary. This can happen especially when we don't have strong duality: the dual optimum then lies exactly on the duality boundary. The challenge then is to modify the optimization algorithm so that the optimization does not get stuck at the duality boundary.
One way of handling this is by using what we call fake sources, which is a type of interior point method. The idea is to modify the dual objective (6) so that the gradient will again push us away from the duality boundary. This is done by introducing extra terms so the dual optimization objective takes the form

$$\mathcal{G}_{fS}(\lambda) = \langle S|\,Z^{ST}Z^{TT-1}Z^{TS}\,|S\rangle + \sum_k \eta_k\,\langle fS_k|\,Z^{TT-1}\,|fS_k\rangle \tag{11}$$

Here the fake source vectors $|fS\rangle$ are set specifically so that $\langle v_1|fS\rangle \neq 0$ as we approach a particular region in the duality boundary. In practice $|fS\rangle$ is taken to be v_1 when we detect that the optimization trajectory of λ is approaching the duality boundary without the dual gradient responding appropriatly. This detection can be done when performing backtracking linesearch to determine the step-size: if after doing the backtracking so we don't exit the domain of duality, we see that the Armijo condition is automatically satisfied, this would be an indication that the gradient is not picking up the boundary information. η_k is the relative magnitude of the fake source term; as we get closer to the dual optimum η_k can be progressively reduced so the fake sources contribute less and less towards the dual objective and the dual objective tends towards the unmodified dual optimum (the tightest dual bound available).