Compact mixed-integer programming relaxations in quadratic optimization

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Abstract. We present a technique for producing valid dual bounds for nonconvex quadratic optimization problems. The approach leverages an elegant piecewise linear approximation for univariate quadratic functions due to Yarotsky \cite{29}, formulating this (simple) approximation using mixed-integer programming. Notably, the number of constraints, binary variables, and auxiliary continuous variables used in this formulation grows logarithmically in the approximation error. Combining this with a diagonal perturbation technique to convert a nonseparable quadratic function into a separable one, we present a mixed-integer convex quadratic relaxation for nonconvex quadratic optimization problems. We study the strength of our formulation in terms of sharpness and the tightness of our approximation. Further, we show that our formulation represents feasible points via a Gray code. We close with computational results on box-constrained quadratic optimization problems, showing that our technique can outperform existing approaches in terms of solve time and dual bounds.

Keywords: Quadratic optimization · Mixed-integer programming

1 Introduction

We are interested in methods to solve optimization problems with quadratic objectives. Consider the following generic problem:

\[ \min_{x \in X} \ h(x) := x^T Q x + c \cdot x \]  \hspace{1cm} (1)

where \( X \subseteq \mathbb{R}^n \) is some nonempty feasible region described by side constraints. When the quadratic objective matrix \( Q \) is not positive semidefinite, this is a difficult nonconvex optimization problem. We will focus on techniques to (approximately) reformulate the nonconvex quadratic objective of (1). Though we do not explicitly consider it in this paper, we note that our techniques can easily be extended to quadratically constrained optimization problems; we leave an analysis and computational experiment of this to future work.

Quadratic optimization problems naturally arise in a number of important applications across science and engineering (see \cite{15,21} and references therein).
In the presence of nonconvexity, such problems are in general very difficult to solve from both a practical and theoretical perspective [20]. As a result, there has been a steady stream of research developing new algorithmic techniques to solve quadratic optimization problems, and variants thereof (see [7] for a survey).

Our approach to approximately solving problems of the form (1) will be to reformulate the objective of (1) using mixed-integer programming (MIP). Given some diagonal matrix $D$, we can equivalently write (1) as

$$\begin{align*}
\min_{x \in X} & \quad h^D(x, y) := x'(Q + D)x + c \cdot x - Dy \\
\text{s.t.} & \quad y_i = x_i^2 \quad \forall i \in [n].
\end{align*}$$

(2a) (2b)

If $D$ is chosen such that $Q + D$ is positive semidefinite, the quadratic constraint will be convex, meaning that all the nonconvexity has been isolated in the univariate quadratic equations $y_i = x_i^2$. This technique is sometimes called “diagonal perturbation” [10]. Our approach hews most closely to that of Dong and Luo [11] and Saxena et al. [22], but we note that diagonal perturbation techniques have been applied throughout the years in a number of settings; for example, convex quadratic [5] or more general nonlinear [13,14] optimization with binary variables, and general nonlinear optimization [1,2,4].

In this work, we present a compact, tight MIP formulation for the graph of a univariate quadratic term: $\{(x, y) \mid l \leq x \leq u, y = x^2\}$. We derive our formulation by adapting an elegant result of Yarotsky [29], who shows that there exists a simple neural network function that approximates $y = x^2$ exponentially well (in terms of the size of the network) over the unit interval. The resulting neural network can be interpreted as a function $F_L : \mathbb{R} \rightarrow \mathbb{R}$ that is build compositionally from a number of simple piecewise linear functions. There is a long and rich strain of research on MIP formulations for piecewise linear functions that serve as approximations for more complex nonlinear functions [8,9,16,17,18,19,26], with recent work focusing particularly on modeling neural networks [3,6,23,24,25].

2 A piecewise linear approximation for univariate quadratic terms

In this section, we present our mixed-integer programming relaxation for (1). We start by describing the construction of Yarotsky, which is a piecewise linear neural network approximation for the univariate quadratic function $F(x) = x^2$. We then formulate the graph of this piecewise linear function using mixed-integer programming, and use it to build a relaxation for the quadratic optimization problem (1). After we derive this formulation, we show that it is a strong (i.e. sharp) representation for our approximation of the quadratic. We then draw an interesting connection between how our formulation represents feasible points through a Gray code: in essence, feasible points are represented in the formulation by their $L$ most significant digits in a binary expansion. Finally, we show that our approximation offers a tight relaxation of the true quadratic function.
2.1 The construction of Yarotsky

For fixed $L \in \mathbb{N}$, recursively define the sawtooth functions $G_i : [0,1] \rightarrow [0,1]$ as

$$G_0(x) = x,$$

$$G_i(x) = \begin{cases} 2G_{i-1}(x) & G_{i-1}(x) < 1/2 \\ 2(1 - G_{i-1}(x)) & G_{i-1}(x) \geq 1/2 \end{cases} \forall i \in \mathbb{N}. $$

Given these functions, Yarotsky observes that

$$F_L(x) := x - \sum_{i=1}^{L} 2^{-2i} G_i(x)$$

approximates the univariate quadratic function $F(x) = x^2$ over the unit input domain $[0,1]$ to within an absolute pointwise error tolerance of $2^{-2L-2}$ [29, Proposition 2].

We include an illustration of $G_L$ and $F_L$ for different values of $L$ in Figure 1(b). Crucially, we will later make use of the fact that $F_L(x) \geq F(x)$ for each $0 \leq x \leq 1$, i.e. $F_L$ is an overestimator for $F$.

2.2 A MIP formulation for $F_L$

We now turn our attention to constructing a mixed-integer programming formulation for $F_L$. As (4) tells us that $F_L$ depends linearly on the sawtooth functions $G_i$, we turn our attention to formulating the piecewise linear equations (3) using MIP.

Furthermore, Yarotsky [29] observes that it is straightforward to represent each of the sawtooth functions as a composition of the standard ReLU activation function $\sigma(x) = \max\{0, x\}$. For example, $G_1(x) = 2\sigma(x) - 4\sigma(x - \frac{1}{2}) + 2\sigma(x - 1)$. In this way, $F_L$ can be written as a neural network with a very particular choice of architecture and weight values.
For the remainder of the section we will use $g_i$ as decision variables in our optimization formulation corresponding to the output of the $i$-th sawtooth function $G_i$. Therefore, $g_0 = x$, and for each of the other sawtooth functions $G_i$ for $i \in [L]$, we introduce a binary decision variable $\alpha_i$. Given some input $x$, these binary variables serve to indicate which piece of the sawtooth the input lies on:

\begin{align}
\alpha_i &= 0 \implies (g_i = 2g_{i-1}) \land (0 \leq g_{i-1} \leq 1/2) \\
\alpha_i &= 1 \implies (g_i = 2(1 - g_{i-1})) \land (1/2 \leq g_{i-1} \leq 1)
\end{align}

Define the set $S_i := \{(g_{i-1}, g_i, \alpha_i) \in [0, 1] \times [0, 1] \times \{0, 1\} \mid (5)\}$ for each $i \in [L]$. It is not difficult to see that a convex hull formulation for $S_i$ is given by

\begin{align}
2(\alpha_i - g_{i-1}) &\leq g_i \leq 2(1 - g_{i-1}), \\
2(g_{i-1} - \alpha_i) &\leq g_i \leq 2g_{i-1}, \\
(g_{i-1}, g_i, \alpha_i) &\in [0, 1] \times [0, 1] \times \{0, 1\}.
\end{align}

Chaining these formulations together for each $i$, we construct a MIP formulation for $G_L := \{(x, y) \in [0, 1] \times [0, 1] \mid y = F_L(x)\}$, the graph of the neural network approximator $F_L$.

**Proposition 1.** Fix some $L \in \mathbb{N}$. A MIP formulation for $(x, y) \in G_L$ is

\begin{align}
g_0 &= x \\
(g_{i-1}, g_i, \alpha_i) &\in S_i \quad i \in [L] \\
y &= x - \sum_{i=1}^{L} 2^{-2i}g_i.
\end{align}

We emphasize that this formulation is extremely compact: it requires only $O(L)$ binary variables, auxiliary continuous variables, and constraints. As noted in Section 2.1, $F_L$ approximates $F$ to within $O(2^{-L})$ pointwise, which implies that the size of our formulation scales logarithmically in the desired accuracy.

It is a straightforward extension of Proposition 1 to consider more general interval domains $x \in [l, u]$ on the inputs. In particular, introducing two auxiliary variables $\tilde{x}, \tilde{y} \in [0, 1]$, we formulate $\tilde{y} = F(\tilde{x}) = \tilde{x}^2$ using (7), and then map them to the $(x, y)$ variables via the linear transformation

$$x = l + (u - l)\tilde{x}, \quad y = l^2 + 2l(u - l)\tilde{x} + (u - l)^2\tilde{y}.$$  

### 2.3 Tying it all together

We are now prepared to construct our mixed-integer programming approximation for (1). For the objective of (1), compute a nonnegative diagonal matrix $D$ such that $Q + D$ is positive semidefinite.\(^4\) Then, for a given $L$, the approximation for (1) is:

\begin{align}
\min_{x \in X, y} &\quad h^D(x, y) \equiv x'(Q + D)x + c \cdot x - Dy \\
\text{s.t.} &\quad (x_i, y_i) \in G_L \quad \forall i \in [n].
\end{align}

\(^4\) This can be accomplished in a number of ways: for example, by computing the minimum eigenvalue of $D$, or by solving a semidefinite programming problem [11].
Using the formulation (7) for the constraint (8b), this yields a mixed-integer convex quadratic reformulation of the problem (ignoring the potential structure of X). This formulation requires at most nL binary variables and $O(nL)$ auxiliary continuous variables and linear constraints. Furthermore, recall that we may set $L = O(\log(1/\epsilon))$ to attain an approximation of accuracy $\epsilon$ for the equations (2b).

Consider any $\hat{x} \in X$, along with any $\hat{y}$ such that $(\hat{x}, \hat{y})$ satisfies (8b). Since $F_L$ overestimates $F$, for each $i \in [n]$, we have $\hat{x}_i^2 \leq \hat{y}_i$. Therefore, $h^D(\hat{x}, \hat{y}) \leq h(\hat{x})$. Since there always will exist such a $\hat{y}$ for any $\hat{x} \in X$, (8) offers a valid dual bound on the optimal cost of (1).

2.4 Formulation strength

The strength of a MIP formulation is a commonly-used metric to assess its potential computational performance. We will show that our proposed formulation is sharp, meaning that its LP relaxation projects to the convex hull of all feasible points. More formally, for a domain $\Gamma \subseteq \mathbb{R}^n$, a formulation $P_L = \{(x, y, z) \in P : z \in \mathbb{Z}^l\}$ for $P \subseteq \mathbb{R}^{n+d+1}$ is valid if $\text{proj}_x(P_L) = \Gamma$. Moreover, it is sharp for $\Gamma$ if $\text{proj}_x(P_L) = \text{conv}(\Gamma)$.

Define $P_L$ as the set given by (7) and let $\Gamma = \text{proj}_{(x,y)}(P_L)$. We wish to show that the formulation $P_L$ is sharp for $\Gamma$.

Theorem 1. The formulation $P_L$ is sharp for $\Gamma$.

Proof. Take $P$ as the LP relaxation of $P_L$ and $R = \text{proj}_{(x,y)}(P)$. For sharpness, we wish to show that $R = \text{conv}(\Gamma)$. Clearly $R \supseteq \text{conv}(\Gamma)$ from validity of our formulation; therefore, we focus on showing that $R \subseteq \text{conv}(\Gamma)$. We start by fixing some $\bar{x} \in [0, 1]$. The result then follows if we can show that the “slice” of $R$ at $\bar{x}$, $R|_{x=\bar{x}} := \{ y \mid (\bar{x}, y) \in R \}$, is contained in $\text{proj}_{x}(\text{conv}(\Gamma))$. Since $R|_{x=\bar{x}} \subseteq [0, 1]$ and is convex, it suffices to show that both its maximum value and minimum value are contained in $\text{conv}(\Gamma)$.

First, let $y^* = \max \{ y \in R|_{x=\bar{x}} \}$. From $R$, we know that $y = x - \sum_{i=1}^{L} 2^{-2i} g_i \leq x$ since $g_i \geq 0$ for all $i$. Hence, $y^* \leq \bar{x}$. Next, we observe that, as $(0,0),(1,1) \in \Gamma$, convexity in turn implies that $(\bar{x}, \bar{x}) \in \text{conv}(\Gamma) \subseteq R$. Therefore, $y^* = \bar{x}$ by maximality, and so $(\bar{x}, y^*) \in \text{conv}(\Gamma)$.

Next, let $y^* = \min \{ y \in R|_{x=\bar{x}} \}$. From definition, it follows that there is some $g^*$ and $\alpha^*$ such that $(\bar{x}, y^*, g^*, \alpha^*) \in P$. Let $G: \mathbb{R} \to \mathbb{R} \text{ by } G(g) = \min \{ 2g, 2(1-g) \}$. If $g_i^* = G(g_{i-1}^*)$ for each $i \in [L]$, then we immediately conclude that there exists some $\alpha^* \in \{0,1\}^L$ such that $(\bar{x}, y^*, g^*, \alpha^*) \in P^I$. This, in turn, implies that $(\bar{x}, y^*) \in \Gamma$.

Otherwise, take $i \in [L]$ as the largest index such that $g_i^* > G(g_{i-1}^*)$. Then, recursively define $\tilde{g}$ such that $\tilde{g}_j = \begin{cases} g_j^* & j < i \\ G(\tilde{g}_{j-1}) & j \geq i \end{cases}$ for each $j \in \{0, \ldots, L\}$. Further, take $\tilde{y} = \bar{x} - \sum_{i=1}^{L} 2^{-2i} \tilde{g}_i$, with $\tilde{\alpha}_i = g_i - 1$ for all $i$, inducing only lower-bounds of 0 on all $g_j$. Then $(\tilde{y}, \bar{x}, \tilde{g}, \tilde{\alpha}) \in R$. We now show that $\tilde{y} < y^*$, contradicting the minimality of $y^*$. 

Compact MIP relaxations in quadratic optimization 5
Let \( \varepsilon = \tilde{g}_i - g^*_i \). Note that \( G: \mathbb{R} \to \mathbb{R} \) is Lipschitz continuous with Lipschitz constant 2. That is, for any \( g, g' \in [0, 1] \), we have that \( |G(g) - G(g')| \leq 2|g - g'| \). Hence, since \( |g^*_i - \tilde{g}_i| \leq \varepsilon \) we conclude inductively that \( |g^*_{i+k} - \tilde{g}_{i+k}| \leq 2^k \varepsilon \) for each \( k \in [L - i] \).

\[
\begin{align*}
y^* - \tilde{y} &= \sum_{i=1}^{L} 2^{-2i}(\tilde{g}_i - g^*_i) \\
&\geq 2^{-2i}(\tilde{g}_i - g^*_i) + \sum_{j=1}^{L} 2^{-2j}2^{j-i} \varepsilon \\
&= 2^{-2i} \varepsilon (1 - 2^i \sum_{j=i+1}^{L} 2^{-j}) \\
&= 2^{-2i} \varepsilon (1 - 2^i (2^{-1} - 2^{-L})) = \varepsilon (2^{-i-L}) > 0
\end{align*}
\]

Therefore, \( \tilde{y} < y^* \), contradicting the minimality of \( y^* \). From this, we conclude that no such \( i \) exists, completing the proof. \( \Box \)

### 2.5 Gray codes and binary representation

We will work with two notions of expressing integers with as vectors in \( \{0, 1\}^L \).

First, we consider the standard binarization with \( L \) bits. That is, for an integer \( t \in \{0, 1, \ldots, 2^L - 1\} \) we define \( \beta^t \in \{0, 1\}^L \) such that \( t = \sum_{j=1}^{L} 2^{L-j} \beta^j \). The reflected Gray code is a binary representation of integers used in computer science that has many convenient properties. The Gray code \( \alpha^t \) of length \( L \) for integer \( t \) can be defined by \( \alpha^t_1 := \beta^t_1 \) and the recursion

\[
\alpha^t_i := \beta^t_i \oplus \beta^t_{i-1} \quad \text{for all } i = 2, \ldots, L, \tag{9}
\]

where we use \( \oplus \) to denote addition modulo 2. By inverting the relation, we obtain

\[
\beta^t_i = \alpha^t_i \oplus \alpha^t_{i-1} \quad \text{for } i = 1, \ldots, L. \tag{10}
\]

Let \( e^k \) denote the standard unit vector that is 1 in the \( k \)th entry and 0 otherwise. For vectors, \( \oplus \) will denote addition modulo 2, componentwise. That is, \( u \oplus v = (u_1 \oplus v_1, \ldots, u_n \oplus v_n) \). Then, for an integer \( t' \), we have that

\[
\alpha^{t'} = \alpha^t \oplus e^k \text{ if and only if } \beta^{t'} = \beta^t \oplus \sum_{i=k}^{L} e^i. \tag{11}
\]

We will show that the binary variables \( \alpha \) in \( P_t \) exactly take on Gray code values. We will establish this connection through the binary representation \( \beta^t \) of integers \( t \).

Let \( X_t^L := (\frac{t}{2^L}, \frac{t+1}{2^L}) \), and let \( X_L := \bigcup_{t=0}^{2^L-1} X_t^L = (0, 1) \setminus \frac{1}{2^L} \mathbb{Z} \). We define the bijections

\[
B_L: X_L \to \{0, 1\}^n \times (0, \frac{1}{2^L}) \text{ such that } x \mapsto (\beta^t, \Delta x) \text{ for } x = 2^{-L}t + \Delta x
\]

\[
A_L: X_L \to \{0, 1\}^n \times (0, \frac{1}{2^L}) \text{ such that } x \mapsto (\alpha, g_L) \text{ via } P_t
\]

Let \( x \in X_t^L \) for some \( t \in \mathbb{Z}^+ \) and let \( (\alpha, g_L) = A(x) \) and \( (\beta, \Delta x) = B_L(x) \). Then \( \beta = \beta^t \). We seek to understand \( \tilde{x} := A^{-1}(\alpha \oplus e^i, g_L) \) in terms of the change in the corresponding \( \beta \). To do so, define the reflection

\[
\rho_{k,L}: \{0, 1\}^L \times (0, \frac{1}{2^L}) \to \{0, 1\}^L \times (0, \frac{1}{2^L}) \text{ as } (\beta, \Delta x) \mapsto (\beta \oplus \sum_{i=k+1}^{L} e^i, 2^{-L} - \Delta x).
\]
In this way, applying $\rho_{k,L}$ corresponds with adding $e^{k+1}$ to the Gray code $\alpha'$ for $\beta$. We will show that $\tilde{x} = B^{-1}_L(\rho_{k-1,L}(\beta, \Delta x))$, via $\mathcal{B}(A^{-1}(\alpha + e^k, g_L)) = \rho_{k-1,L}(\beta, \Delta x)$. That is, we will show that adding $e^k$ to $\alpha$ corresponds with adding $e^i$ to $\alpha'$. Thus, as $\alpha = \alpha' = 0$ when $x \in (0, 2^{-L})$, we must have $\alpha = \alpha'$.

Note that for $\alpha_i \in \{0,1\}$, case analysis can be transformed into an equation as

$$g_i = \begin{cases} 2g_{i-1} & \alpha_i = 0 \\ 2(1 - g_{i-1}) & \alpha_i = 1 \end{cases} \Leftrightarrow g_i = (1 - 2\alpha_i)(2g_{i-1} - 1) + 1. \quad (12)$$

**Theorem 2.** Let $x \in X^t_L \subseteq (0,1)$ with $t \in \mathbb{Z}_+$. Let $(x,y,g,\alpha) \in P_I$. Then $\alpha$ is the reflected Gray code for $t$, i.e., $\alpha = \alpha'$.

**Proof.** First note that if $x \in (0, \frac{1}{2^t})$ (i.e., $x \in X^t_L$), then $A_L(x) = B_L(x) = (0, x)$. Furthermore, by definition $\alpha^0 = \beta^0 = 0$. Thus, for $t = 0$, the result holds.

Let $x \in X^t_L$, $(\alpha, g_L) = A_L(x)$, and $(\beta, \Delta x) = B_L(x)$. We will show that the analogous relation to (11) holds for $\alpha$. The result will then follow from induction from the $\alpha = \beta = 0$ case.

Thus, let $\alpha' = \alpha + e^t$, and $\tilde{x} = A^{-1}_L(\alpha', g_L)$. Let $\beta'$ be such that $\tilde{x} \in X^t_L$, and $(\tilde{\beta}, \Delta \tilde{x}) = B_L(\tilde{x})$, so that $\beta = \beta'$ and $\beta = \beta'$. We will show $(\tilde{\beta}, \Delta \tilde{x}) = \rho_{i-1,L}(\beta, \Delta x)$, which implies that the analogous relation to (11) holds.

Let $\tilde{y}$ and $\tilde{g}$ be such that $(\tilde{x}, \tilde{y}, \tilde{g}, \tilde{\alpha}) \in P_I$. Note that this choice is unique. We compute $(\beta, \Delta \tilde{x})$ by recursively computing the binary representation for each $g_j$, until we reach $\tilde{g}_0 = \tilde{x}$. For each $j \leq i - 1$, let $(\gamma_j, \Delta g_j) = B_{L-j}(g_j)$ and $(\tilde{\gamma}_j, \Delta \tilde{g}_j) = B_{L-j}(\tilde{g}_j)$. Here, $\gamma_j, \gamma_j \in \{0,1\}^{L-j}$. By definition, $(\beta, \Delta x) = (\gamma_0, \Delta g_0)$ and $(\tilde{\beta}, \Delta \tilde{x}) = (\tilde{\gamma}_0, \Delta \tilde{g}_0)$.

Note that, since $\tilde{g}_L = g_L$ and $\tilde{\alpha}_j = \alpha_j$ fixes $g_j$ based on $g_{j-1}$ via (12) for all $j \geq i+1$, we have $g_j = \tilde{g}_j$ for all $j = i, i+1, \ldots, L$.

We will show by induction that for all $j = 0, \ldots, i - 1$, we have

$$(\tilde{\gamma}_j, \Delta \tilde{g}_j) = \rho_{i-j-1,L-j}(\gamma_j, \Delta g_j). \quad (13)$$

Hence, the proof is completed by showing that this holds for $j = 0$. We start the induction at $j = i - 1$, and then proceed by decreasing $j$.

**Base case:** We first show that $g_{i-1} = 1 - \tilde{g}_{i-1}$. To see this, we express $g_i$ and $\tilde{g}_i$ via (12). Then, after simplification with $g_i = \tilde{g}_i$ and $\tilde{\alpha}_i = 1 - \alpha_i$, we obtain $\tilde{g}_{i-1} = 1 - g_{i-1}$, yielding

$$\tilde{g}_{i-1} = 1 - \left(\sum_{k=1}^{L-i+1} 2^{-k}\gamma_{i-1,k} + \Delta g_{i-1}\right)
= 1 - \sum_{k=1}^{L-i+1} 2^{-k} - 2^{-(L-i+1)} + \sum_{k=1}^{L-i+1} 2^{-k}(1 - \gamma_{i-1,k}) + (2^{-(L-i+1)} - \Delta g_{i-1})
= \sum_{k=1}^{L-i+1} 2^{-k}(1 - \gamma_{i-1,k}) + (2^{-(L-i+1)} - \Delta g_{i-1}).$$

Thus $\gamma_i = \gamma_i + \sum_{k=1}^{i} e^k$, yielding $(\gamma_i, \Delta \gamma_i) = \rho_{0,L-i+1}(\gamma_i, \Delta g_i)$.

**Induction step:** We now assume that (13) holds for $i$, and prove for the $j - 1$ case.

We introduce operations $\mathcal{O}_\alpha : \{0,1\}^L \times \mathbb{R} \rightarrow \{0,1\}^{L+1} \times \mathbb{R}$, for $\tilde{L} = L - j$, relating $(\gamma_j, \Delta g_j)$ with $(\gamma_{j-1}, \Delta g_{j-1})$ given $\alpha_j = \alpha$. 
Operations $O_\alpha$. For $g \in [0,1]$ be written in binary form with $\hat{L} - 1$ bits, that is, $g = \sum_{k=1}^{\hat{L}-1} 2^{-k} \gamma_k + \Delta g$ for $\gamma \in \{0,1\}^{\hat{L}-1}$. The operation $O_\alpha$ maps $(\gamma, \Delta g) \mapsto (\gamma', \Delta g')$ where $g' = \sum_{k=1}^{\hat{L}} 2^{-k} \gamma'_k + \Delta g'$, for some $\Delta g' \in [0,2^{-\hat{L}})$. Notice that the output has one addition bit than the input. We define these maps for $\alpha = 0$ and $\alpha = 1$.

Operation $O_0$: Let $g' = \frac{1}{2} g$ and define $\gamma' \in \{0,1\}^L$ by $g' = \sum_{k=1}^{\hat{L}} 2^{-k} \gamma'_k + \Delta g'$.

\[
g' = \frac{1}{2} g = \frac{1}{2} \left( \sum_{k=1}^{\hat{L}-1} 2^{-k} \gamma_k + \Delta g \right) = 0 \cdot 2^{-1} + \sum_{k=2}^{\hat{L}} 2^{-k} \gamma_{k-1} + \frac{1}{2} \Delta g.\]

Thus $\gamma'_1 = 0$ and $\gamma'_k = \gamma_{k-1}$ for $k = 2, \ldots, L$, with $\Delta g' = \frac{1}{2} \Delta g$.

Operation $O_1$: Let $g' = 1 - \frac{1}{2} g$ and define $\gamma' \in \{0,1\}^L$ by $g' = \sum_{k=1}^{\hat{L}} 2^{-k} \gamma'_k + \Delta g'$. Then

\[
g' = 1 - \frac{1}{2} g = 1 - \frac{1}{2} \left( \sum_{k=1}^{\hat{L}-1} 2^{-k} \gamma_k + \Delta g \right) = 1 - \sum_{k=1}^{\hat{L}-1} 2^{-k} \gamma_k - \frac{1}{2} \Delta g = 1 - \sum_{k=2}^{\hat{L}} 2^{-k} \gamma_{k-1} - \frac{1}{2} \Delta g
\]

\[
= 1 - \sum_{k=1}^{\hat{L}-1} 2^{-k} - 2^{-L} + \sum_{k=2}^{\hat{L}} 2^{-k}(1 - \gamma_{k-1}) + \frac{1}{2}(2^{-L} - \Delta g)
\]

\[
= 1 \cdot 2^{-1} + \sum_{k=2}^{\hat{L}} 2^{-k}(1 - \gamma_{k-1}) + \frac{1}{2}(2^{-L} - \Delta g)
\]

Thus, $\gamma'_1 = 1$ and $\gamma'_k = 1 - \gamma_{k-1}$ for $k = 2, \ldots, \hat{L}$, with $\Delta g' = \frac{1}{2}(2^{-L} - \Delta g)$.

Induction case analysis. Now, define $(\gamma_{j-1}, \Delta g_{j-1})$ as in (13). Then we have $(\gamma_{j-1}, \Delta g_{j-1}) = O_\alpha(\gamma_j, \Delta g_j)$ and $(\gamma'_{j-1}, \Delta g'_{j-1}) = O_\alpha(\gamma'_j, \Delta g'_j)$. Thus, since the same operation is applied bitwise, with $\gamma_{j,k} = 1 - \gamma_{j,k}$ for $k \geq i - j$, $\gamma_{j,k} = \gamma_{j,k}$ for $k \leq i - j - 1$, and by definition of the operation $\gamma_{j-1,k} = \gamma_{j,k}$ for $k \leq i - j - 1$, we have that $\gamma'_{j-1,k} = 1 - \gamma'_{j-1,k}$ for $k \geq i - j + 1$ and $\gamma'_{j,k} = \gamma_{j,k}$ for $k \leq i - j$, as desired.

To deal with $\Delta g_{j-1}$, we now consider two cases.

Case 1: $\alpha_j = 0$. In this case, we have

\[
\Delta g_{j-1} = \frac{1}{2} \Delta g_j = \frac{1}{2} (2^{-(L-j)} - \Delta g_j) = \frac{1}{2} (2^{-(L-j)} - 2 \Delta g_{j-1}) = 2^{-(L-(j-1))} - \Delta g_{j-1}
\]

Thus, $(\bar{g}_{j-1}, \Delta g_{j-1}) = r_{i-j,L-j+1}(g_{j-1}, \Delta g_{j-1})$, as desired.

Case 2: $\alpha_j = 1$. In this case, we have

\[
\Delta g_{j-1} = \frac{1}{2} (2^{-(L-(j-1))} - \Delta g_{j-1}) = \frac{1}{2} (2^{-(L-(j-1))} - 2 \Delta g_{j-1}) = 2^{-(L-j)} - 2 \Delta g_{j-1}
\]

Thus, $(\bar{g}_{j-1}, \Delta g_{j-1}) = r_{i-j,L-j+1}(g_{j-1}, \Delta g_{j-1})$, as desired. 

A connection with existing MIP formulations. Interestingly, Gray codes also naturally appear in the “logarithmic” MIP formulations for general continuous univariate piecewise linear functions due to Vielma et al. [27,28]. Consider
applying this existing formulation\(^5\) to approximate the univariate quadratic term with the same \(2^L + 1\) breakpoints as discussed in Section 2.5. The resulting MIP formulation is uses \(L\) binary variables, which follow the same interpretation as the neural network formulation as discussed in Theorem 2. Moreover, it requires \(\mathcal{O}(L)\) linear constraints (excluding variable) bounds, and is ideal, a stronger property than the sharpness shown in Theorem 1. However, it comes at the price of an additional \(2^L + 1\) auxiliary continuous variables, and so is unlikely to be practical without a careful handling through, e.g., column generation. Therefore, our formulation sacrifices strength to reduce this to \(\mathcal{O}(L)\) auxiliary continuous variables.

### 2.6 Area comparisons

Instead of overapproximating \(y = x^2\), we can relax the equation with a union of polytopes. This can be achieved with \((6)\), \(0 \leq y \leq x \leq 1, y \leq x - \sum_{i=1}^{L} \frac{g_i}{2^{2i}}\), \(y \geq 2x - 1\) and

\[
y \geq \left(x - \sum_{i=1}^{j} \frac{g_i}{2^{2i}}\right) - \frac{1}{2^{2j+2}} \quad j \in 0, \ldots, L.
\]

Table 1 compares the volume of our relaxed method with the method of Dong and Luo \([11]\) on the interval \(x \in [-2, 1]\). As \(L\) increases, the volume of our relaxation consistently shrinks by a factor of 4, which is strictly greater by a fair margin to the improvement rate observed for the method of Dong and Luo. We can formalize our rate of improvement in the following proposition.

| Method | \(L = 0\) | \(L = 1\) | \(L = 2\) | \(L = 3\) | \(L = 4\) |
|--------|-----------|-----------|-----------|-----------|-----------|
| CDA    | 6.75      | 1.94 (3.47) | 0.659 (2.95) | 0.1970 (3.34) | 0.0530 (3.72) |
| R-NN   | 5.06      | 1.27 (4)   | 0.316 (4)  | 0.0791 (4)  | 0.0198 (4)  |

Table 1: Volume comparison for R-NN, the relaxation of our method, and CDA, the method of Dong and Luo \([11]\). Factor of improvement over the previous value for \(L\) is shown in bold.

**Proposition 2.** The volume of our approximation decreases by a factor of 4 with each subsequent layer (i.e. as \(L\) increases). Furthermore, the expected error at points \(x\) sampled uniformly at random from the input interval domain is proportional to the total volume.

\(^5\) In actuality, any Gray code yields a (potentially distinct) logarithmic formulation for a univariate function. Here, we mean the one constructed with the reflected Gray code, which is the most common choice regardless.
3 A computational study

We study the efficacy of our MIP relaxation approach on a family box constrained quadratic objective (boxQP) optimization problem instances:

\[
\min_{0 \leq x \leq 1} \; x^T Q x + c \cdot x
\]

Despite its simple constraint structure, this is a nonconvex optimization problem when \( Q \) is not positive semidefinite, and is difficult from both a theoretical and a practical perspective.

We compare 5 methods:

1. **GRB**: The nonconvex quadratic optimization method in Gurobi v9.1.0.
2. **GRB3**: The same as **GRB**, with parameter \texttt{MIPFocus=3} (“best bound focus”).
3. **BRN**: Baron v20.4.14, using CPLEX v12.10 for the MIP/LP solver.
4. **CDA**: The algorithm of Dong and Luo [11]. We select \( \nu = 3 \) (i.e. three binary variables) for each univariate quadratic term. Gurobi v9.1.0 is the MIP solver with “best bound focus”.
5. **NN**: The new formulation (7). We select \( L = 3 \) for each univariate quadratic term. Gurobi v9.1.0 is the MIP solver with “best bound focus”.

Note that we have selected the \( \nu \) parameter in **CDA** and the \( L \) parameter in **NN** such that both methods will end up using the same number of binary variables for each instance. Our objective in this computational study is to measure the quality of the dual bound provided by the different methods. To place the methods on an even footing on the primal side, as initialization we run the nonconvex quadratic optimization method in Gurobi v9.1.0 with “feasible solution emphasis” to produce a good starting feasible solution. We then inject this primal objective bound as a “cut-off” for each method.

We implement each model in the JuMP algebraic modeling language [12]. For both **NN** and **CDA**, we use Mosek v9.2.2 to solve a semidefinite programming
problem to produce the “tightest” diagonal matrix $D$ such that $Q + D$ is positive semidefinite (see Dong and Luo [11] for details). Each method is provided a time limit of 5 minutes. Computational experiments are performed on a machine with a 2.4 GHz CPU with 8 cores and 16 GB of RAM. Our code is publicly available at https://github.com/joehuchette/compact-mips-for-qp.

We compare these three algorithms on 105 boxQP instances as studied in Dong and Luo [11]. We split these instances into three families: 71 “solved” instances on which each method terminates at optimality within the time limit, 15 “unsolved” instances on which each method terminates due to the time limit, and 19 “contested” instances on which some methods terminate and some do not.

We present the computational results in Table 2, stratified by family. We consider 4 metrics:

- **time**: The shifted geometric mean of the solve time in seconds (shift is minimum solve time in the family).
- **gap**: The shifted geometric mean of the final relative optimality gap $\frac{|db - bpb|}{|bpb|}$, where $db$ is the dual bound provided by the method and $bpb$ is the best observed primal solution for the instance across all methods. Shift is taken as $\max\{10^{-4}, \text{minimum gap observed in the family}\}$.
- **BB**: The number of instances in which the method either produced the best dual bound, or attained Gurobi’s default optimality criteria of $\text{gap} < 10^{-4}|bpb|$. Note that on a given instance, more than one method can potentially attain the best bound.
- **TO**: The number of instances in which the solver times out and terminates due to the time limit.

We note that even if the solver terminates within the time limit (with an “optimal” solver status), the optimality gap for NN or CDA as reported in Table 2 may be nonzero, due to the fact that these two methods serve as relaxations for the original boxQP problem. We leave as future work an implementation that iteratively refines the approximation to guarantee a pre-specified approximation error, as done by Dong and Luo [11]. We summarize the results of our computational study in Table 2. At a high level, we observe that NN attains the “best bound” on 97 of 105 instances. It runs more quickly than other methods on solved instances, and is the clear winner in terms of bound quality on the unsolved instances. We now survey each family in more detail.

**Solved instances** On the solved instances, all methods are able to terminate quickly—all in under a second, on average. Despite being a relaxation, the bound from NN meets Gurobi’s default termination criteria on each of the 71 instances. We note that this cannot be taken for granted, as CDA is unable to meet this bar on 23 of 71 instances (though we stress again that this is a “static” formulation; with refinement, this gap can be reduced, though potentially at greater computational cost).
Contested instances The native algorithm in Gurobi performs best on the contested instances, on which it is able to terminate within the time limit on 18 of 19. NN is able to meet the gap criteria on 13 of 19 instances, though it times out on a bit more than half. From this, we conclude that on 4 instances, NN did not terminate due to optimality, but nonetheless had a dual bound which would certify optimality, meaning the deficiency was on the primal side. We omit averaged solve times from the table as the values are confounded by the arbitrarily set time limit. Taken together, we conclude that there is a transitional family of instances wherein Gurobi is still able to solve to optimality, but all other methods succumb to the curse of dimensionality.

Unsolved instances This family of instances tests the scenario where a method is given a fixed time budget and is asked to produce the best possible dual bound. On these 15 instances, NN is the clear winner, producing the best bounds on 13 and the lowest average gap. CDA is closest in terms of average gap, but is never the best method on any one instance. BRN produces somewhat worse bounds on average, while GRB and GRB3 lag far behind. Note that we do not include the “time” or “TO” columns as they provide no new additional information (each method on each instance in this family times out at 5 minutes).

Other preliminary experimental observations We summarize additional experiments that we do not include fully in the interest of space. We performed a similar series of experiments where the objective was transformed by replacing the objective with an “epigraph” variable \( y \) that is constrained such that \( y \geq x'Qx + c \cdot x \). In other words, the nonconvex quadratic objective is replaced

| family | method | time | gap | 71/71 | TO |
|--------|--------|------|-----|-------|----|
| solved | GRB    | 0.38 | 0.00% | 71/71 | -  |
|        | GRB3   | 0.72 | 0.00% | 71/71 | -  |
|        | BRN    | 0.47 | 0.00% | 71/71 | -  |
|        | CDA    | 0.67 | 0.08% | 48/71 | -  |
|        | NN     | 0.20 | 0.01% | 71/71 | -  |

| contested | GRB | 0.00% | 18/19 | 1/19 |
|           | GRB3| -     | 18/19 | 1/19 |
|           | BRN | 0.04% | 9/19  | 10/19|
|           | CDA | 0.87% | 6/19  | 14/19|
|           | NN  | 0.15% | 13/19 | 10/19|

| unsolved  | GRB | -18.89% | 9/15  | -  |
|           | GRB3| -15.45%  | 2/15  | -  |
|           | BRN | -7.17%   | 9/15  | -  |
|           | CDA | -3.47%   | 9/15  | -  |
|           | NN  | -2.05%   | 13/15 | -  |

Table 2: Computational results. Solve time reported in seconds.

Nonetheless, we can offer some qualitatively observations: that GRB ran faster than GRB3, and that otherwise solve time correlated strongly with the number of timeouts.
with a nonconvex quadratic constraint. The relative performance is nearly identical, though BRN exhibits a severe degradation in performance, particularly on the unsolved instances. We also performed preliminary computations with CPLEX v12.10 as the “base” solver instead of Gurobi, but performance was generally close, albeit somewhat slower.

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