Spectral relaxations for global optimization of mixed-integer quadratic programs

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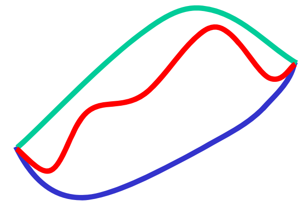
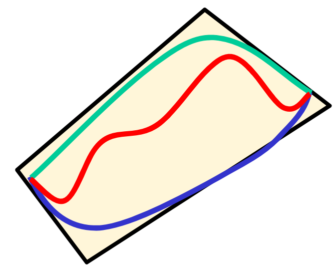
Joint work with Carlos Nohra and Arvind Raghunathan

BARON'S RELAXATIONS

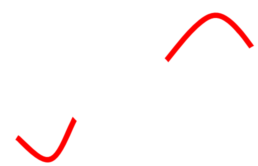
- **Nonlinear outer approximations of factorable functions**
  - Ryoo and Sahinidis (1995)



- **Polyhedral outer approximations**
  - Tawarmalani and Sahinidis (2005)



- **Some nonlinear relaxations**
  - Khajavirad and Sahinidis (2018)
    - *Original NLP becomes convex*
  - Nohra, Raghunathan and Sahinidis (2021)
    - *Original NLP does not become convex*



This talk

- **Dynamic relaxation selection**
  - LP, NLP, MIP

PROBLEM FORMULATION

- **We consider mixed-integer quadratic programs (MIQPs) of the form:**

$$
\begin{aligned}
\min_x \quad & x^T Q x + q^T x \\
\text{s.t.} \quad & Ax = b \\
& Cx \leq d \\
& l \leq x \leq u \\
& x_i \in \mathbb{Z}, \quad \forall i \in I \subseteq \{1, \ldots, n\}
\end{aligned}
$$

where $Q \in \mathbb{R}^{n \times n}$ is a symmetric matrix which may be indefinite and $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$, $C \in \mathbb{R}^{p \times n}$, $d \in \mathbb{R}^p$

- **Inequalities handled but not exploited**

BASIC RELAXATION APPROACHES

- **Factorable programming relaxations (McCormick, 1976)**

Introduce new variables

$$X_{ij} = x_i x_j,\ i,j = 1,\ldots,n$$

$$q_{ij} \neq 0$$

$$\longrightarrow$$

$$\boxed{\begin{aligned} X_{ij} &\geq u_i x_j + u_j x_i - u_i u_j \\ X_{ij} &\geq l_i x_j + l_j x_i - l_i l_j \\ X_{ij} &\leq u_i x_j + l_j x_i - u_i l_j \\ X_{ij} &\leq l_i x_j + u_j x_i - l_i u_j \end{aligned}}$$

McCormick inequalities

- **Reformulation Linearization Technique (RLT) relaxations (Sherali and Adams 1990, 1992)**

Reformulation step: construct reformulated problem by adding **redundant nonlinear constraints**

Linearization step: linearize reformulated problem by **introducing new variables**

- **Semidefinite programming relaxations (Shor, 1987)**

Introduce symmetric matrix of new variables

$$X = xx^T \longrightarrow \boxed{X - xx^T \succcurlyeq 0}$$

Semidefinite constraint

Loss of sparsity; quadratic increase in number of variables

REFORMULATION-BASED APPROACHES

- **Eigenvalue reformulation (Rosen et al., 1987)**

$$Q = U\Lambda U^T = \sum_{i=1}^{n} \lambda_i u_i u_i^T$$

λ_i : i-th eigenvalue of Q

u_i : eigenvector associated with the i-th eigenvalue of Q

  - **Use eigendecomposition of the quadratic matrix to construct a convex quadratic relaxation**
  - **Resulting relaxation yields very weak bounds**

- **Undominated d.c. decompositions of quadratic functions (Bomze and Locatelli, 2004)**

$$\min_{x \in P} \; x^T Q x + q^T x = f(x) - g(x) \qquad f(x) = x^T (Q - B) x + q^T x \qquad g(x) = x^T B x$$

The matrix B is chosen such that $B \succcurlyeq 0$ and $Q - B \succcurlyeq 0$

An SDP-based algorithm is proposed in order to find B

- **Quadratic convex reformulations for binary quadratic programs (Billionnet et al., 2009, 2013)**
  - **Reformulate original problem into another one whose continuous relaxation is convex**
  - **Perturbation parameters used to construct the reformulated problem obtained by solving certain SDPs**

EIGENVALUE RELAXATION

Original problem

$$\min_x \; x^T Q x + q^T x$$
$$\text{s.t. } Ax = b, \quad Cx \le d, \quad l \le x \le u, \quad x_i \in \mathbb{Z}, \; \forall i \in I \subseteq \{1, \ldots, n\} \qquad \text{(MIQP)}$$

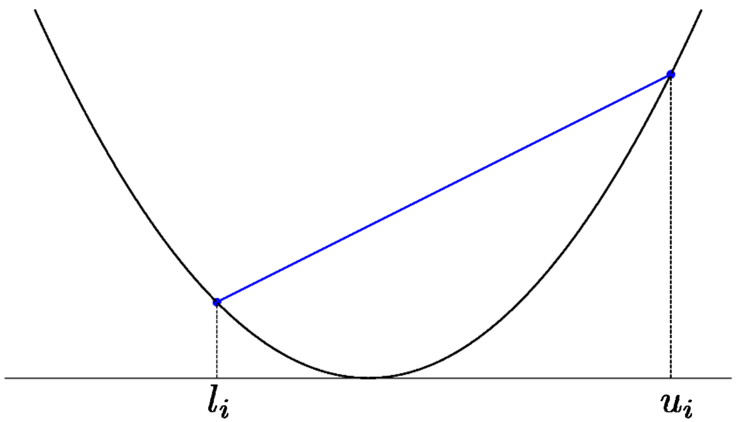
Reformulated problem

$$\min_x \; x^T Q x + q^T x + \alpha_e \sum_{i=1}^{n} x_i^2 - \alpha_e \sum_{i=1}^{n} \boxed{x_i^2}$$
$$\text{s.t. } Ax = b, \quad Cx \le d, \quad l \le x \le u, \quad \boxed{x_i \in \mathbb{Z}, \; \forall i \in I \subseteq \{1, \ldots, n\}}$$
$$\text{where } \alpha_e \ge 0$$

Relax using concave envelope

Relax integrality conditions

The concave envelope of x_i^2 over $[l_i, u_i]$ is given by the line $(l_i + u_i)x_i - l_i u_i$



EIGENVALUE RELAXATION

Original problem

$$\begin{aligned} \min_x \;& x^T Q x + q^T x \\ \text{s.t. } & Ax = b, \quad Cx \le d, \quad l \le x \le u, \quad x_i \in \mathbb{Z}, \; \forall i \in I \subseteq \{1, \ldots, n\} \end{aligned} \qquad \text{(MIQP)}$$

Quadratic relaxation

$$\begin{aligned} \min_x \;& x^T Q x + q^T x + \alpha_e \sum_{i=1}^{n} x_i^2 - \alpha_e \sum_{i=1}^{n} ((l_i + u_i) x_i - l_i u_i) \\ \text{s.t. } & Ax = b, \quad Cx \le d, \quad l \le x \le u \end{aligned} \qquad \text{(EIG)}$$

where $\alpha_e \ge 0$

EIGENVALUE RELAXATION

Original problem

$$\begin{aligned} \min_x \;& x^T Q x + q^T x \\ \text{s.t. }& Ax = b, \quad Cx \le d, \quad l \le x \le u, \quad x_i \in \mathbb{Z}, \;\; \forall i \in I \subseteq \{1,\dots,n\} \end{aligned} \qquad \text{(MIQP)}$$

Quadratic relaxation

$$\begin{aligned} \min_x \;& x^T (Q + \alpha_e I_n) x + (q - \alpha_e (l+u))^T x + \alpha_e l^T u \\ \text{s.t. }& Ax = b, \quad Cx \le d, \quad l \le x \le u \end{aligned} \qquad \text{(EIG)}$$

where $\alpha_e \ge 0$

To ensure convexity of this relaxation, we must choose α_e **such that** $Q + \alpha_e I_n \succcurlyeq 0$

This is equivalent to choosing $\alpha_e \ge -\min(0, \lambda_{\min}(Q))$

The tightest convex relaxation of form (EIG) **for which** $Q + \alpha_e I_n \succcurlyeq 0$ **is obtained by setting** $\alpha_e = -\min(0, \lambda_{\min}(Q))$

Under this approach, we convexify the objective function of (MIQP) **by perturbing the diagonal elements of the matrix** Q

EIGENVALUE RELAXATION

Original problem

$$\begin{aligned} \min_x \quad & x^T Q x + q^T x \\ \text{s.t.} \quad & Ax = b, \quad Cx \le d, \quad l \le x \le u, \quad x_i \in \mathbb{Z}, \ \forall i \in I \subseteq \{1, \dots, n\} \end{aligned} \qquad \text{(MIQP)}$$

Quadratic relaxation

$$\begin{aligned} \min_x \quad & x^T (Q + \alpha_e I_n) x + (q - \alpha_e (l + u))^T x + \alpha_e l^T u \\ \text{s.t.} \quad & Ax = b, \quad Cx \le d, \quad l \le x \le u \end{aligned} \qquad \text{(EIG)}$$

where $\alpha_e = -\min(0, \lambda_{\min}(Q))$

Remarks:

- **Hammer and Rubin (1970) is one of the earliest works considering convexification methods based on the smallest eigenvalue of the quadratic matrix**
- **The construction of this relaxation can be seen as an application of d.c. programming methods (Tuy, 1995) or alphaBB techniques (Androulakis et al., 1995)**
- **Despite its simplicity, the eigenvalue relaxation can provide significantly tight bounds**

EIGENVALUE RELAXATION

- **Proposition 1:**

Assume that the matrix Q is indefinite. Let $\alpha_e = -\lambda_{\min}(Q)$. Then, we have:

$$\mu_{\text{EIG}} := \min_{x} \; x^T Q_{\alpha_e} x + q_{\alpha_e}^T x + k_{\alpha_e} \qquad \text{(EIG)}$$
$$\text{s.t.} \;\; Ax = b, \quad Cx \le d, \quad l \le x \le u$$
$$\text{where } Q_{\alpha_e} = Q + \alpha_e I_n$$
$$q_{\alpha_e} = q - \alpha_e (l + u)$$
$$k_{\alpha_e} = \alpha_e l^T u$$

$$\Longleftrightarrow$$

$$\mu_{\text{SDP\_EIG}} := \min_{x,X} \; \langle Q, X \rangle + q^T x \qquad \text{(SDP\_EIG)}$$
$$\text{s.t.} \;\; Ax = b, \quad Cx \le d, \quad l \le x \le u$$
$$X - xx^T \succcurlyeq 0$$
$$\langle I_n, X \rangle - (l+u)^T x + l^T u = 0$$

GENERALIZED EIGENVALUE RELAXATION

Original problem

$$\min_x \; x^T Q x + q^T x$$
$$\text{s.t.} \;\; Ax = b, \quad Cx \le d, \quad l \le x \le u, \quad x_i \in \mathbb{Z}, \;\; \forall i \in I \subseteq \{1,\dots,n\} \qquad \text{(MIQP)}$$

Reformulated problem

$$\min_x \; x^T Q x + q^T x + \boxed{\alpha_g}\sum_{i=1}^{n} x_i^2 - \boxed{\alpha_g}\sum_{i=1}^{n} x_i^2 + \boxed{\alpha_g}\|Ax-b\|^2$$
$$\text{s.t.} \;\; Ax = b, \quad Cx \le d, \quad l \le x \le u, \quad x_i \in \mathbb{Z}, \;\; \forall i \in I \subseteq \{1,\dots,n\}$$

where $\alpha_g \ge 0$

Use the same perturbation parameter for the x_i^2 terms and the term $\|Ax-b\|^2$

GENERALIZED EIGENVALUE RELAXATION

Original problem

$$\min_{x} \; x^T Q x + q^T x$$
$$\text{s.t.} \;\; Ax = b, \quad Cx \le d, \quad l \le x \le u, \quad x_i \in \mathbb{Z}, \;\; \forall i \in I \subseteq \{1, \ldots, n\} \qquad \text{(MIQP)}$$

Reformulated problem

$$\min_{x} \; x^T Q x + q^T x + \alpha_g \sum_{i=1}^{n} x_i^2 - \alpha_g \sum_{i=1}^{n} \boxed{x_i^2} + \alpha_g \|Ax - b\|^2$$
$$\text{s.t.} \;\; Ax = b, \quad Cx \le d, \quad l \le x \le u, \quad \boxed{x_i \in \mathbb{Z}, \;\; \forall i \in I \subseteq \{1, \ldots, n\}}$$
where $\alpha_g \ge 0$

Relax using concave envelope

Relax integrality conditions

GENERALIZED EIGENVALUE RELAXATION

Original problem

$$\begin{aligned} \min_{x} \;\; & x^T Q x + q^T x \\ \text{s.t.} \;\; & Ax = b, \quad Cx \le d, \quad l \le x \le u, \quad x_i \in \mathbb{Z}, \;\; \forall i \in I \subseteq \{1, \dots, n\} \end{aligned} \qquad \text{(MIQP)}$$

Quadratic relaxation

$$\begin{aligned} \min_{x} \;\; & x^T Q x + q^T x + \alpha_g \sum_{i=1}^{n} x_i^2 - \alpha_g \sum_{i=1}^{n} ((l_i + u_i) x_i - l_i u_i) + \alpha_g \|Ax - b\|^2 \\ \text{s.t.} \;\; & Ax = b, \quad Cx \le d, \quad l \le x \le u \end{aligned} \qquad \text{(GEIG)}$$

where $\alpha_g \geq 0$

GENERALIZED EIGENVALUE RELAXATION

Original problem

$$\min_x \; x^T Q x + q^T x \qquad \text{(MIQP)}$$
$$\text{s.t.} \;\; Ax = b, \quad Cx \le d, \quad l \le x \le u, \quad x_i \in \mathbb{Z}, \;\; \forall i \in I \subseteq \{1, \ldots, n\}$$

Quadratic relaxation

$$\min_x \; x^T \left(Q + \alpha_g \left(I + A^T A\right)\right) x + \left(q - \alpha_g \left(2A^T b + l + u\right)\right)^T x + \alpha_g \left(l^T u + b^T b\right) \qquad \text{(GEIG)}$$
$$\text{s.t.} \;\; Ax = b, \quad Cx \le d, \quad l \le x \le u$$

where $\alpha_g \ge 0$

To ensure convexity of this relaxation, we must choose α_g **such that** $Q + \alpha_g \left(I + A^T A\right) \succcurlyeq 0$

- **Proposition 2**

Let $\alpha_g \ge -\min(0, \lambda_{\min}(Q, I_n + A^T A))$. Then, (GEIG) is a **convex quadratic program.**

The tightest convex relaxation of form (GEIG) **for which** $Q + \alpha_g \left(I + A^T A\right) \succcurlyeq 0$ **is obtained by setting** $\alpha_g = -\min(0, \lambda_{\min}(Q, I_n + A^T A))$

GENERALIZED EIGENVALUE RELAXATION

- **Proposition 3:**

Consider the eigenvalue relaxation and the generalized eigenvalue relaxation

$$\begin{aligned} \mu_{\text{EIG}} := \min_x \;& x^T Q_{\alpha_e} x + q_{\alpha_e}^T x + k_{\alpha_e} \qquad \text{(EIG)} \\ \text{s.t.}\;& Ax = b, \quad Cx \le d, \quad l \le x \le u \\ \text{where}\;& Q_{\alpha_e} = Q + \alpha_e I_n \\ & q_{\alpha_e} = q - \alpha_e(l + u) \\ & k_{\alpha_e} = \alpha_e l^T u \end{aligned}$$

$$\begin{aligned} \mu_{\text{GEIG}} := \min_x \;& x^T Q_{\alpha_g} x + q_{\alpha_g}^T x + k_{\alpha_g} \qquad \text{(GEIG)} \\ \text{s.t.}\;& Ax = b, \quad Cx \le d, \quad l \le x \le u \\ \text{where}\;& Q_{\alpha_g} = Q + \alpha_g \left(I + A^T A\right) \\ & q_{\alpha_g} = q - \alpha_g \left(2A^T b + l + u\right) \\ & k_{\alpha_g} = \alpha_g \left(l^T u + b^T b\right) \end{aligned}$$

Let $\alpha_e = -\min(0, \lambda_{\min}(Q))$ in (EIG) and $\alpha_g = -\min(0, \lambda_{\min}(Q, I_n + A^T A))$ in (GEIG). Then, the **generalized eigenvalue relaxation** is **at least as tight** as the **eigenvalue relaxation**, i.e., $\mu_{\text{GEIG}} \ge \mu_{\text{EIG}}$.

GENERALIZED EIGENVALUE RELAXATION

- **Proposition 4:**

Assume that the matrix Q is indefinite. Let $\alpha_g = -\lambda_{\min}(Q, I_n + A^T A)$. Then, we have:

$$\begin{aligned} \mu_{\text{GEIG}} := \min_x \ & x^T Q_{\alpha_g} x + q_{\alpha_g}^T x + k_{\alpha_g} \quad \text{(GEIG)} \\ \text{s.t. } & Ax = b, \quad Cx \le d, \quad l \le x \le u \\ \text{where } & Q_{\alpha_g} = Q + \alpha_g \left(I + A^T A\right) \\ & q_{\alpha_g} = q - \alpha_g \left(2A^T b + l + u\right) \\ & k_{\alpha_g} = \alpha_g \left(l^T u + b^T b\right) \end{aligned}$$

$$\Longleftrightarrow$$

$$\begin{aligned} \mu_{\text{SDP\_GEIG}} := \min_{x,X} \ & \langle Q, X \rangle + q^T x \quad \text{(SDP\_GEIG)} \\ \text{s.t. } & Ax = b, \quad Cx \le d, \quad l \le x \le u \\ & X - xx^T \succcurlyeq 0 \\ & \langle I_n + A^T A, X \rangle - \left(l + u + 2A^T b\right)^T x + l^T u + b^T b = 0 \end{aligned}$$

EIGENVALUE RELAXATION IN THE NULLSPACE OF A

Original problem

$$\begin{aligned} \min_x \ & x^T Q x + q^T x \\ \text{s.t.} \ & Ax = b, \quad Cx \le d, \quad l \le x \le u, \quad x_i \in \mathbb{Z}, \ \forall i \in I \subseteq \{1, \ldots, n\} \end{aligned} \qquad \text{(MIQP)}$$

Quadratic relaxation

$$\begin{aligned} \min_x \ & x^T (Q + \alpha_z I_n) x + (q - \alpha_z (l + u))^T x + \alpha_z l^T u \\ \text{s.t.} \ & Ax = b, \quad Cx \le d, \quad l \le x \le u \end{aligned} \qquad \text{(EIGNS)}$$

where $\alpha_z \ge 0$

This relaxation has the same form as the eigenvalue relaxation, but in this case α_z is determined by making use of the nullspace of A

- **Proposition 5**

> Denote by Z an orthonormal basis for the nullspace of the matrix A. Let $\alpha_z \ge -\min(0, \lambda_{\min}(Z^T Q Z))$. Then, (EIGNS) is a **convex quadratic program.**

The tightest convex relaxation of form (EIGNS) is obtained by setting
$\alpha_z = -\min(0, \lambda_{\min}(Z^T Q Z))$

EIGENVALUE RELAXATION IN THE NULLSPACE OF A

- **Proposition 6:**

Consider the generalized eigenvalue relaxation and the eigenvalue relaxation in the nullspace of A

$$\begin{aligned} \mu_{\text{GEIG}} := \min_x \ & x^T Q_{\alpha_g} x + q_{\alpha_g}^T x + k_{\alpha_g} \qquad \text{(GEIG)} \\ \text{s.t.} \ & Ax = b, \quad Cx \le d, \quad l \le x \le u \\ \text{where } Q_{\alpha_g} &= Q + \alpha_g \left(I + A^T A\right) \\ q_{\alpha_g} &= q - \alpha_g \left(2A^T b + l + u\right) \\ k_{\alpha_g} &= \alpha_g \left(l^T u + b^T b\right) \end{aligned}$$

$$\begin{aligned} \mu_{\text{EIGNS}} := \min_x \ & x^T Q_{\alpha_z} x + q_{\alpha_z}^T x + k_{\alpha_z} \qquad \text{(EIGNS)} \\ \text{s.t.} \ & Ax = b, \quad Cx \le d, \quad l \le x \le u \\ \text{where } Q_{\alpha_z} &= Q + \alpha_z I_n \\ q_{\alpha_z} &= q - \alpha_z (l + u) \\ k_{\alpha_z} &= \alpha_z l^T u \end{aligned}$$

Let $\alpha_g = -\min(0, \lambda_{\min}(Q, I_n + A^T A))$ in (GEIG) and $\alpha_z = -\min(0, \lambda_{\min}(Z^T Q Z))$ in (EIGNS). Then, the **eigenvalue relaxation in the nullspace** of A is **at least as tight** as the **generalized eigenvalue relaxation**, i.e., $\mu_{\text{EIGNS}} \ge \mu_{\text{GEIG}}$.

EIGENVALUE RELAXATION IN THE NULLSPACE OF A

- **Proposition 7:**

Assume that the matrix Z^TQZ is indefinite. Let $\alpha_z = -\lambda_{\min}(Z^TQZ)$. Then, we have:

$$
\begin{aligned}
\mu_{\text{EIGNS}} := \min_{x} \;& x^TQ_{\alpha_z}x + q_{\alpha_z}^T x + k_{\alpha_z} \quad \text{(EIGNS)}\\
\text{s.t.}\;& Ax = b, \quad Cx \le d, \quad l \le x \le u\\
\text{where } & Q_{\alpha_z} = Q + \alpha_z I_n\\
& q_{\alpha_z} = q - \alpha_z(l+u)\\
& k_{\alpha_z} = \alpha_z l^T u
\end{aligned}
$$

$$\Longleftrightarrow$$

$$
\begin{aligned}
\mu_{\text{SDP\_EIGNS}} := \min_{x,X} \;& \langle Q, X\rangle + q^T x \quad \text{(SDP\_EIGNS)}\\
\text{s.t.}\;& Ax = b, \quad Cx \le d, \quad l \le x \le u\\
& X - xx^T \succcurlyeq 0\\
& \langle I_n, X\rangle - (l+u)^T x + l^T u = 0\\
& \langle A^TA, X\rangle - \left(2A^Tb\right)^T x + b^Tb = 0
\end{aligned}
$$

DETERMINING Z^TQZ

To determine Z^TQZ we need to:

1. Calculate the nullspace basis Z. This can be done through a QR factorization which requires $\mathcal{O}(n^3)$ FLOPS.

2. Compute Z^TQZ, which is the projection of Q onto the nullspace of A. This also requires $\mathcal{O}(n^3)$ FLOPS.

Question:
Can we obtain a good approximation of $\lambda_{\min}(Z^TQZ)$ without explicitly calculating Z ?

EIGENVALUE RELAXATION IN THE NULLSPACE OF A

- **Proposition 8**

Let δ be a real scalar. Then, the following hold:

(a) If the matrix Q is indefinite, $\lambda_{\min}(Q, I_n + \delta A^T A)$ is a strictly increasing function of δ for $\delta \geq 1$.

(b) $\lim_{\delta\to\infty} \lambda_{\min}(Q, I_n + \delta A^T A) = \min(0, \lambda_{\min}(Z^T Q Z))$.

This proposition implies that we can obtain a good approximation of the bound given by the eigenvalue relaxation in the nullspace of the equality constraints

$$\begin{aligned} \min_x \ & x^T (Q + \alpha_z I_n) x + (q - \alpha_z (l+u))^T x + \alpha_z l^T u \\ \text{s.t.} \ & Ax = b, \quad Cx \leq d, \quad l \leq x \leq u \end{aligned} \qquad \text{(EIGNS)}$$

where $\alpha_z = -\min(0, \lambda_{\min}(Z^T Q Z))$

by solving the following quadratic program

$$\begin{aligned} \min_x \ & x^T Q x + q^T x + \alpha(\delta)(x^T x - (l+u)^T x + l^T u) + \boxed{\alpha(\delta)\cdot\delta\cdot\|Ax-b\|^2} \\ \text{s.t.} \ & Ax = b, \quad Cx \leq d, \quad l \leq x \leq u \end{aligned} \qquad (\text{QP}(\delta))$$

where $\alpha(\delta) = -\lambda_{\min}(Q, I_n + \delta A^T A)$

This term vanishes for any feasible x

We can drop this term and still have a convex quadratic relaxation

for a sufficiently large value of δ

SPECTRAL RELAXATIONS

$$\mu_{\text{EIG}} := \min_x \; x^T Q_{\alpha_e} x + q_{\alpha_e}^T x + k_{\alpha_e} \quad \text{(EIG)}$$
$$\text{s.t.} \;\; Ax = b, \quad Cx \le d, \quad l \le x \le u$$
$$\text{where } Q_{\alpha_e} = Q + \alpha_e I_n$$
$$q_{\alpha_e} = q - \alpha_e (l + u)$$
$$k_{\alpha_e} = \alpha_e l^T u$$
$$\alpha_e = -\lambda_{\min}(Q)$$

$\Longleftrightarrow$

$$\mu_{\text{SDP\_EIG}} := \min_{x,X} \; \langle Q, X \rangle + q^T x \quad \text{(SDP\_EIG)}$$
$$\text{s.t.} \;\; Ax = b, \quad Cx \le d, \quad l \le x \le u$$
$$X - xx^T \succcurlyeq 0$$
$$\langle I_n, X \rangle - (l+u)^T x + l^T u = 0$$

$$\mu_{\text{GEIG}} := \min_x \; x^T Q_{\alpha_g} x + q_{\alpha_g}^T x + k_{\alpha_g} \quad \text{(GEIG)}$$
$$\text{s.t.} \;\; Ax = b, \quad Cx \le d, \quad l \le x \le u$$
$$\text{where } Q_{\alpha_g} = Q + \alpha_g \left(I + A^T A\right)$$
$$q_{\alpha_g} = q - \alpha_g \left(2A^T b + l + u\right)$$
$$k_{\alpha_g} = \alpha_g \left(l^T u + b^T b\right)$$
$$\alpha_g = -\lambda_{\min}(Q, I_n + A^T A)$$

$\Longleftrightarrow$

$$\mu_{\text{SDP\_GEIG}} := \min_{x,X} \; \langle Q, X \rangle + q^T x \quad \text{(SDP\_GEIG)}$$
$$\text{s.t.} \;\; Ax = b, \quad Cx \le d, \quad l \le x \le u$$
$$X - xx^T \succcurlyeq 0$$
$$\langle I_n + A^T A, X \rangle - \left(l + u + 2A^T b\right)^T x + l^T u + b^T b = 0$$

$$\mu_{\text{EIGNS}} := \min_x \; x^T Q_{\alpha_z} x + q_{\alpha_z}^T x + k_{\alpha_z} \quad \text{(EIGNS)}$$
$$\text{s.t.} \;\; Ax = b, \quad Cx \le d, \quad l \le x \le u$$
$$\text{where } Q_{\alpha_z} = Q + \alpha_z I_n$$
$$q_{\alpha_z} = q - \alpha_z (l + u)$$
$$k_{\alpha_z} = \alpha_z l^T u$$
$$\alpha_z = -\lambda_{\min}(Z^T Q Z)$$

$\Longleftrightarrow$

$$\mu_{\text{SDP\_EIGNS}} := \min_{x,X} \; \langle Q, X \rangle + q^T x \quad \text{(SDP\_EIGNS)}$$
$$\text{s.t.} \;\; Ax = b, \quad Cx \le d, \quad l \le x \le u$$
$$X - xx^T \succcurlyeq 0$$
$$\langle I_n, X \rangle - (l+u)^T x + l^T u = 0$$
$$\langle A^T A, X \rangle - \left(2A^T b\right)^T x + b^T b = 0$$

$$\mu_{\text{EIGNS}} \ge \mu_{\text{GEIG}} \ge \mu_{\text{EIG}}$$

IMPLEMENTATION IN BARON

- Incorporated spectral relaxations in the global optimization solver BARON
  - BARON's default portfolio of relaxations:
    - LP relaxations
    - Convex NLP relaxations
    - MILP relaxations
  - Expanded BARON's portfolio of relaxations by adding the spectral relaxations
    - New QP relaxations invoked at nonconvex nodes
    - Eigenvalue and generalized eigenvalue problems solved with LAPACK
    - Convex QP relaxations solved with CPLEX
  - Implemented dynamic relaxation selection strategy
    - Switches between polyhedral and quadratic relaxations throughout the tree based on their relative strength (similar to Khajavirad and Sahinidis, 2018)
- Developed spectral branching rule
  - Increase the impact of branching decisions on the bounds given by the spectral relaxations

SPECTRAL BRANCHING

$$\min_x \; x^T Q x + q^T x \quad \text{s.t.} \; x \in \{0,1\}^n$$

$$Q = \begin{bmatrix} 0 & 26 & 44 & -73 \\ 26 & 0 & -45 & 11 \\ 44 & -45 & 0 & 84 \\ -73 & 11 & 84 & 0 \end{bmatrix} \qquad q = \begin{bmatrix} -119 \\ 27 \\ -187 \\ -2 \end{bmatrix}$$

$$\min_x \; x^T Q x + q^T x + \alpha_e \sum_{i=1}^{n} (x_i^2 - x_i) \quad \text{(EIG)}$$
$$\text{s.t.} \; x \in [0,1]^n$$
$$\text{where } \alpha_e = -\lambda_{\min}(Q)$$

Root node: $\lambda_{\min}(Q) = -149.8$ **Set of branching candidates:** $\mathcal{B} = \{1,2,3,4\}$

Branch on the variable that leads to the largest increase in the smallest eigenvalue of the quadratic matrix

Branch on x_1:
$$\hat{Q}_1 = \begin{bmatrix} 0 & -45 & 11 \\ -45 & 0 & 84 \\ 11 & 84 & 0 \end{bmatrix}$$

Branch on x_2:
$$\hat{Q}_2 = \begin{bmatrix} 0 & 44 & -73 \\ 44 & 0 & 84 \\ -73 & 84 & 0 \end{bmatrix}$$

Branch on x_3:
$$\hat{Q}_3 = \begin{bmatrix} 0 & 26 & -73 \\ 26 & 0 & 11 \\ -73 & 11 & 0 \end{bmatrix}$$

Branch on x_4:
$$\hat{Q}_4 = \begin{bmatrix} 0 & 26 & 44 \\ 26 & 0 & -45 \\ 44 & -45 & 0 \end{bmatrix}$$

Spectral branching with complete enumeration (requires the solution of $|\mathcal{B}|$ eigenvalue problems)

$\lambda_{\min}(\hat{Q}_1) = -100.2$ $\lambda_{\min}(\hat{Q}_2) = -135.3$ $\lambda_{\min}(\hat{Q}_3) = -81.5$ $\boxed{\lambda_{\min}(\hat{Q}_4) = -77.3}$

Approximation 1: Use Gershgorin's Circle Theorem (GCT) to obtain a lower bound estimate for $\lambda_{\min}(\hat{Q}_i)$

$\underline{\lambda}_{\min}^{\text{GCT}}(\hat{Q}_1) = -129$ $\underline{\lambda}_{\min}^{\text{GCT}}(\hat{Q}_2) = -157$ $\underline{\lambda}_{\min}^{\text{GCT}}(\hat{Q}_3) = -99$ $\boxed{\underline{\lambda}_{\min}^{\text{GCT}}(\hat{Q}_4) = -89}$

SPECTRAL BRANCHING

$$\min_x \; x^TQx + q^Tx \quad \text{s.t.} \; x \in \{0,1\}^n$$

$$Q = \begin{bmatrix} 0 & 26 & 44 & -73 \\ 26 & 0 & -45 & 11 \\ 44 & -45 & 0 & 84 \\ -73 & 11 & 84 & 0 \end{bmatrix} \qquad q = \begin{bmatrix} -119 \\ 27 \\ -187 \\ -2 \end{bmatrix}$$

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Branch on x_2:

$$\hat{Q}_2 = \begin{bmatrix} 0 & 44 & -73 \\ 44 & 0 & 84 \\ -73 & 84 & 0 \end{bmatrix}$$

Branch on x_3:

$$\hat{Q}_3 = \begin{bmatrix} 0 & 26 & -73 \\ 26 & 0 & 11 \\ -73 & 11 & 0 \end{bmatrix}$$

Branch on x_4:

$$\hat{Q}_4 = \begin{bmatrix} 0 & 26 & 44 \\ 26 & 0 & -45 \\ 44 & -45 & 0 \end{bmatrix}$$

Spectral branching with complete enumeration (requires the solution of $|\mathcal{B}|$ eigenvalue problems)

$\lambda_{\min}(\hat{Q}_1) = -100.2$ $\lambda_{\min}(\hat{Q}_2) = -135.3$ $\lambda_{\min}(\hat{Q}_3) = -81.5$ $\boxed{\lambda_{\min}(\hat{Q}_4) = -77.3}$

Approximation 2: Let v be the eigenvector corresponding to $\lambda_{\min}(Q)$

Select as branching variable the one corresponding to the entry of v with the largest magnitude

The eigenvector corresponding to $\lambda_{\min}(Q)$ is given by $v = \begin{bmatrix} 0.50 \\ -0.30 \\ -0.56 \\ \boxed{0.58} \end{bmatrix}$

TEST SET

– **960 Cardinality Binary Quadratic Programs (CBQPs) by Lima and Grossmann (2016)**

$$\begin{aligned} \min_{x} \quad & x^T Q x + q^T x \\ \text{s.t.} \quad & \sum_{i=1}^{n} x_i = M, \\ & x_i \in \{0,1\},\ \ i = 1,\ldots,n \end{aligned}$$

$Q \in \mathbb{R}^{n\times n}$ **indefinite**

$M \in \{n/5, n/1.25\}$

Number of variables: $n \in \{50, 75, 100, 200, 300, 400\}$

Density of the quadratic matrix: $\rho \in \{0.10, 0, 50, 0.75, 1.00\}$

Entries of Q and q randomly generated from uniform distributions over the intervals $[-1,1], [0,1], [-100,100], [0,100]$

– **315 Equality-constrained Integer Quadratic Programs (EIQPs) generated similar to Billionnet et al.**

$$\begin{aligned} \min_{x\in\mathbb{R}^n} \quad & x^T Q x + q^T x \\ \text{s.t.} \quad & Ax = b, \\ & x_i \in \{0,1\},\ \ i = 1,\ldots,n \end{aligned}$$

With up to 400 variables

Problems available from ftp://ftp.merl.com/pub/raghunathan/MIQP-TestSet/*

COMPARISON BETWEEN RELAXATIONS

- **Eigenvalue relaxation (EIG)**
- **Generalized eigenvalue relaxation (GEIG)**
- **Eigenvalue relaxation in the nullspace of the equality constraints (EIGNS)**
- **Level-1 Reformulation Linearization Technique relaxation (RLT)**
- **Semidefinite programming relaxations:**

(SDPd)

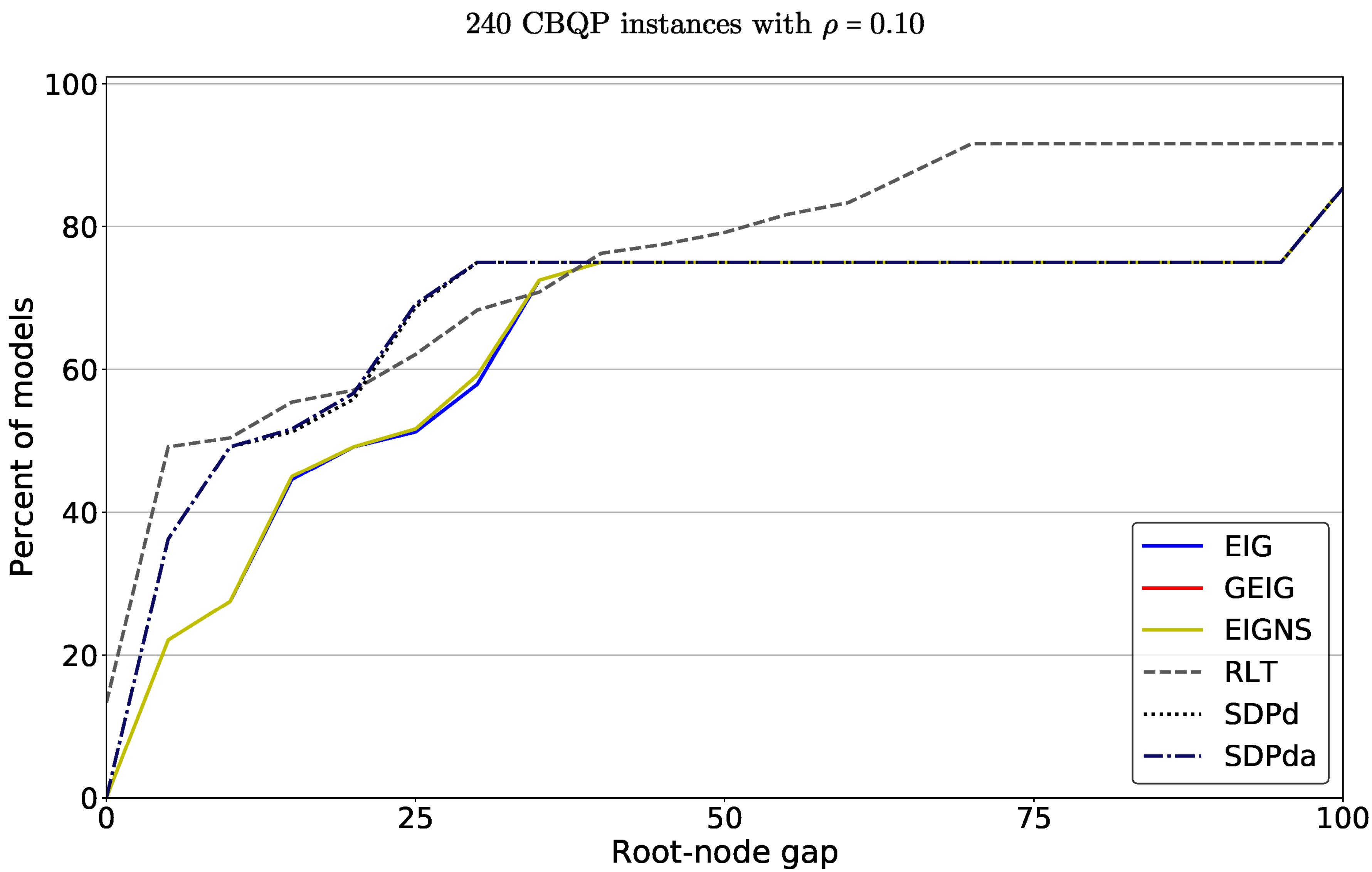
$$
\begin{aligned}
\min_{x,X} \quad & \langle Q, X \rangle + q^T x \\
\text{s.t.} \quad & Ax = b, \quad Cx \leq d, \quad l \leq x \leq u \\
& X - xx^T \succcurlyeq 0 \\
& X_{ii} \leq u_i x_i + l_i x_i - u_i l_i, \; i = 1, \ldots, n
\end{aligned}
$$

(SDPda)

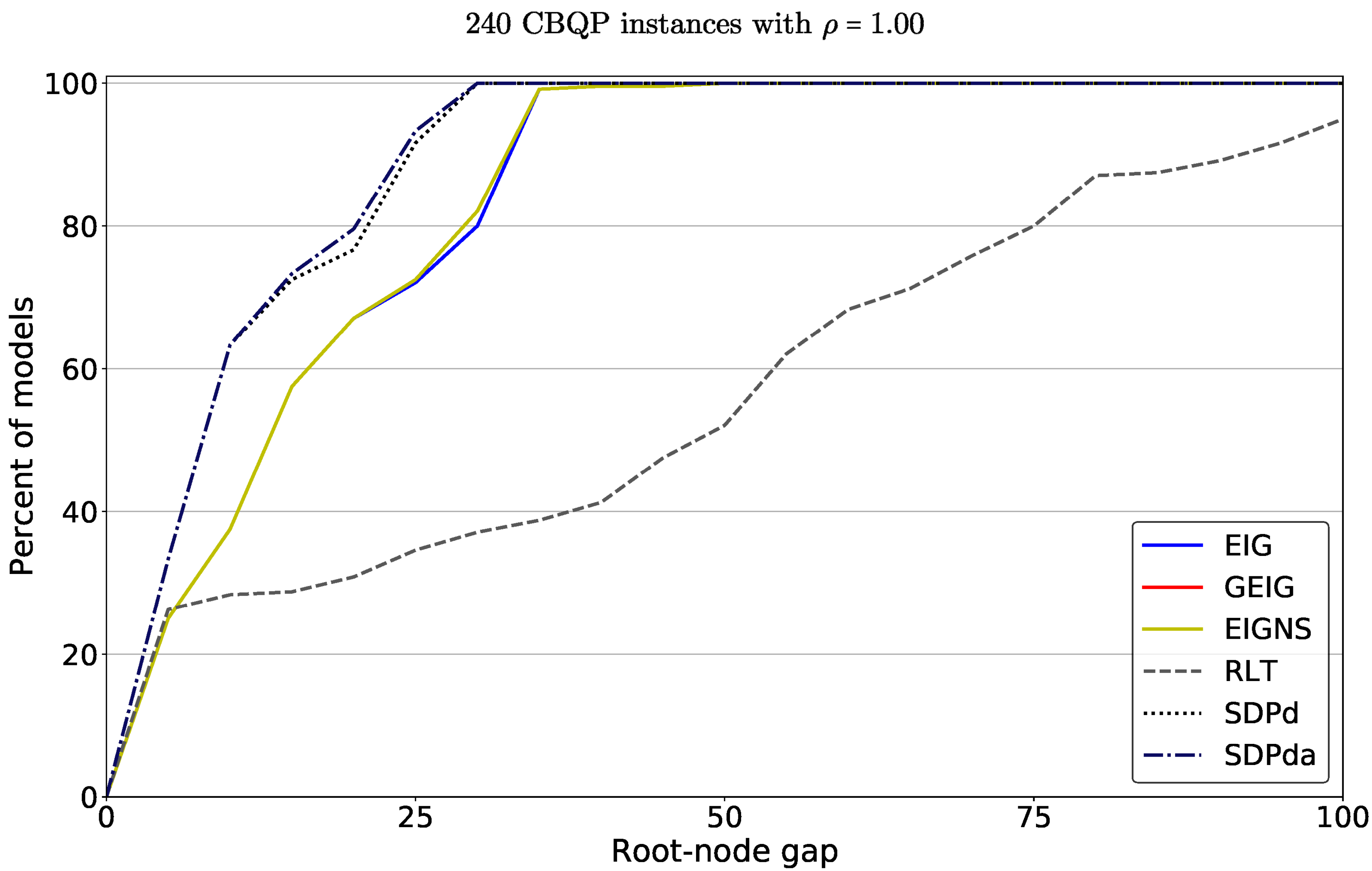
$$
\begin{aligned}
\min_{x,X} \quad & \langle Q, X \rangle + q^T x \\
\text{s.t.} \quad & Ax = b, \quad Cx \leq d, \quad l \leq x \leq u \\
& X - xx^T \succcurlyeq 0 \\
& X_{ii} \leq u_i x_i + l_i x_i - u_i l_i, \; i = 1, \ldots, n \\
& \langle A^T A, X \rangle - 2(A^T b)^T x + b^T b = 0
\end{aligned}
$$

- **Solvers:**
  - **LP and QP relaxations: CPLEX 12.9 under GAMS**
  - **SDP relaxations: SDPT3 4.0 under MATLAB**

COMPARISON BETWEEN RELAXATIONS



COMPARISON BETWEEN RELAXATIONS



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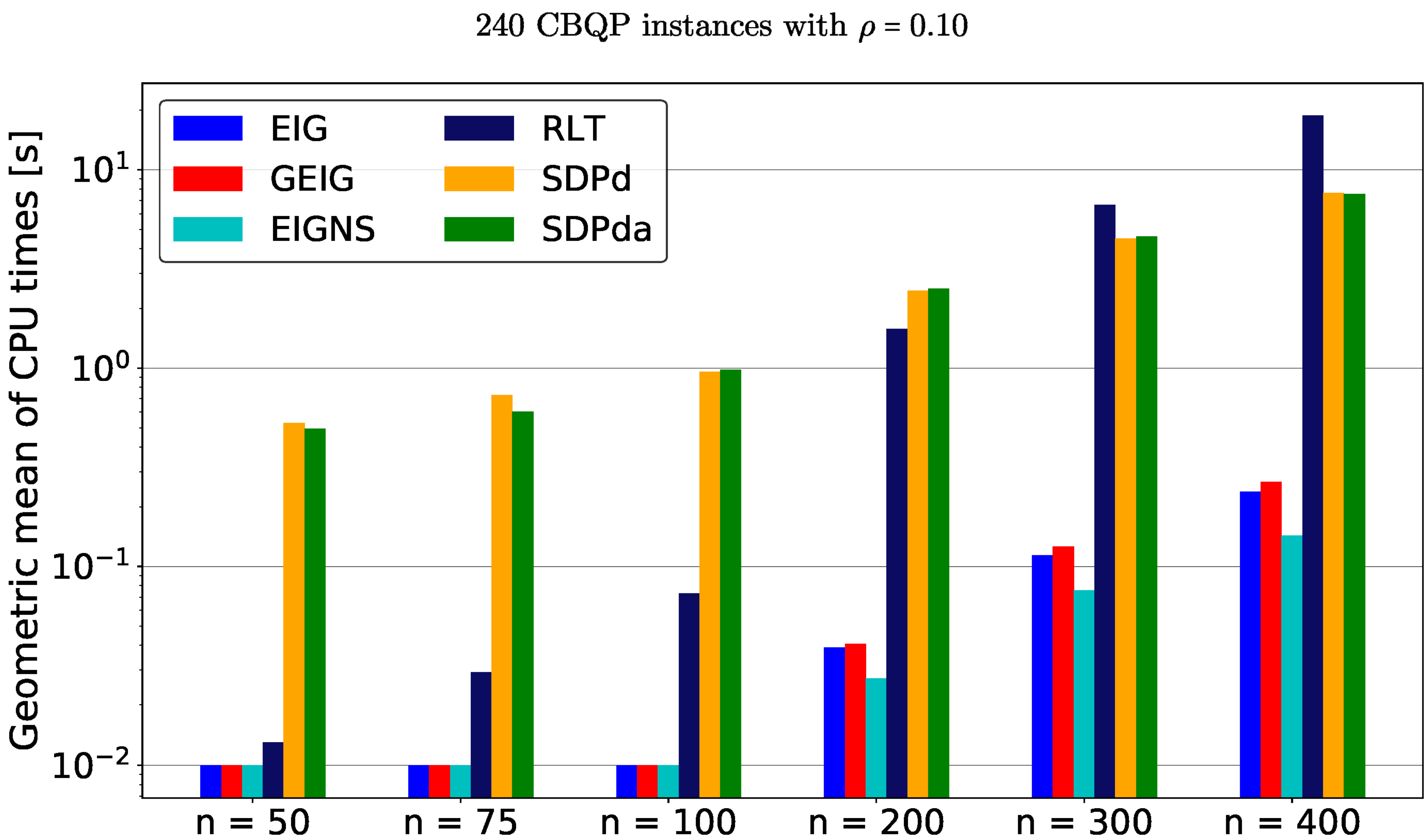
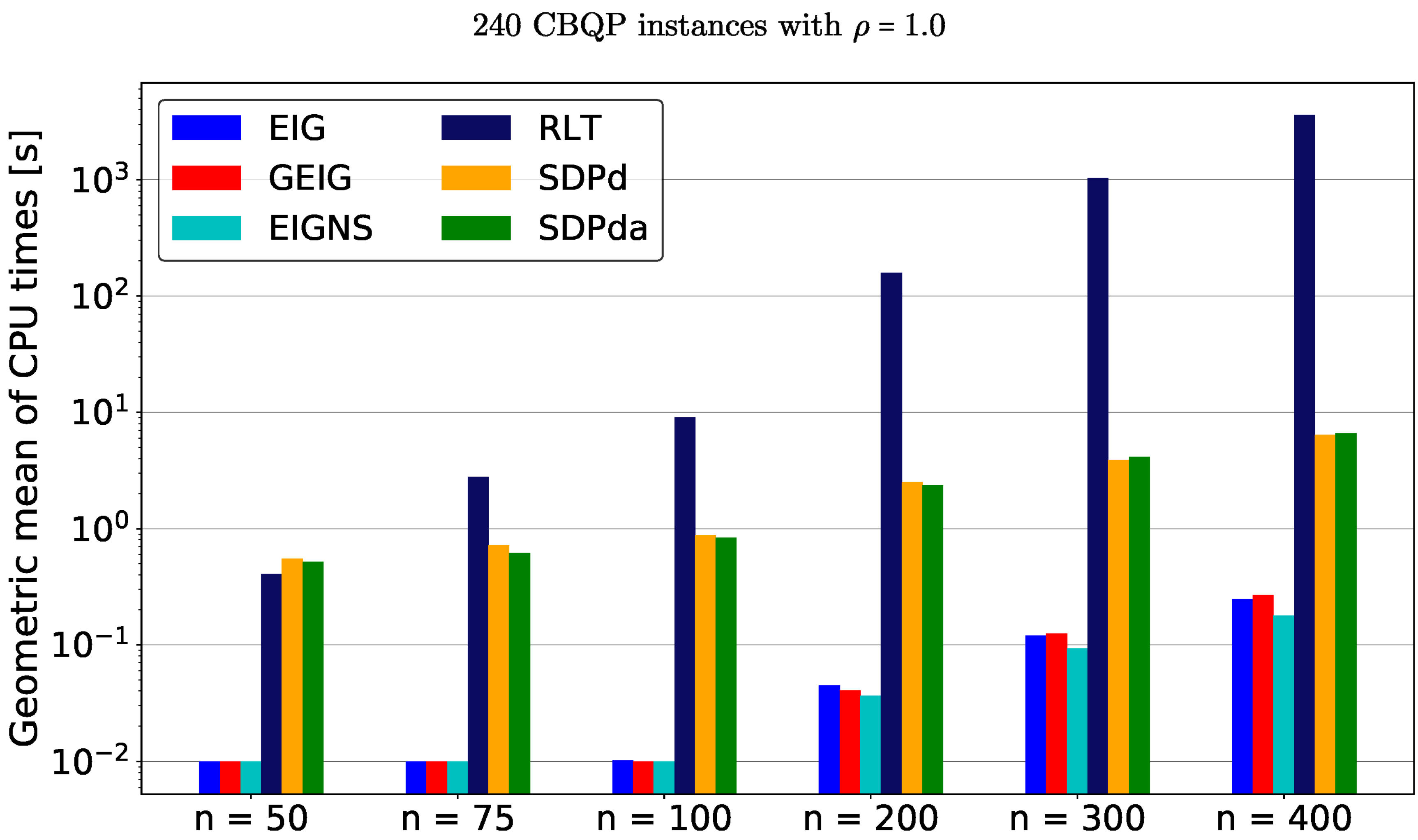
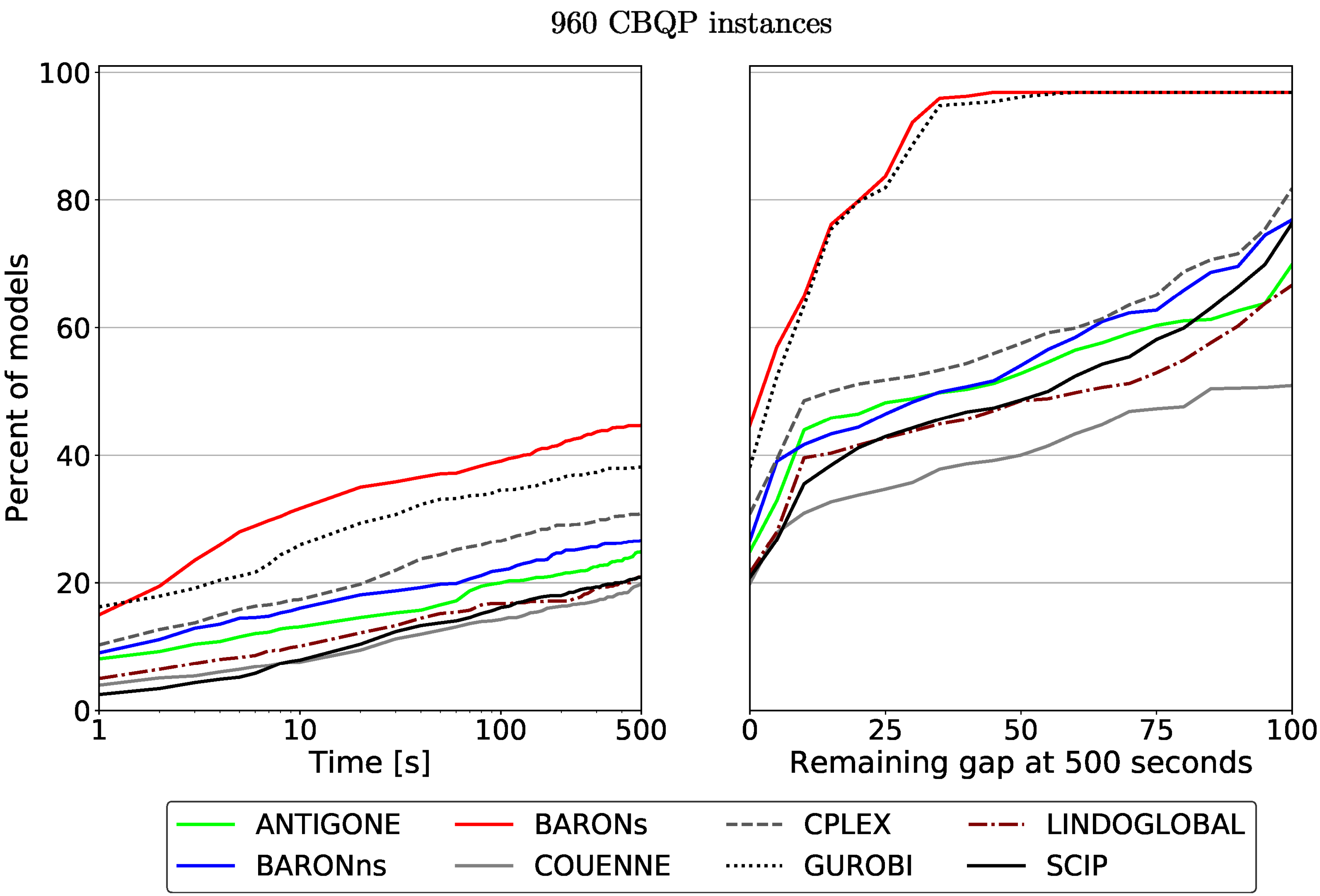


COMPARISON BETWEEN RELAXATIONS

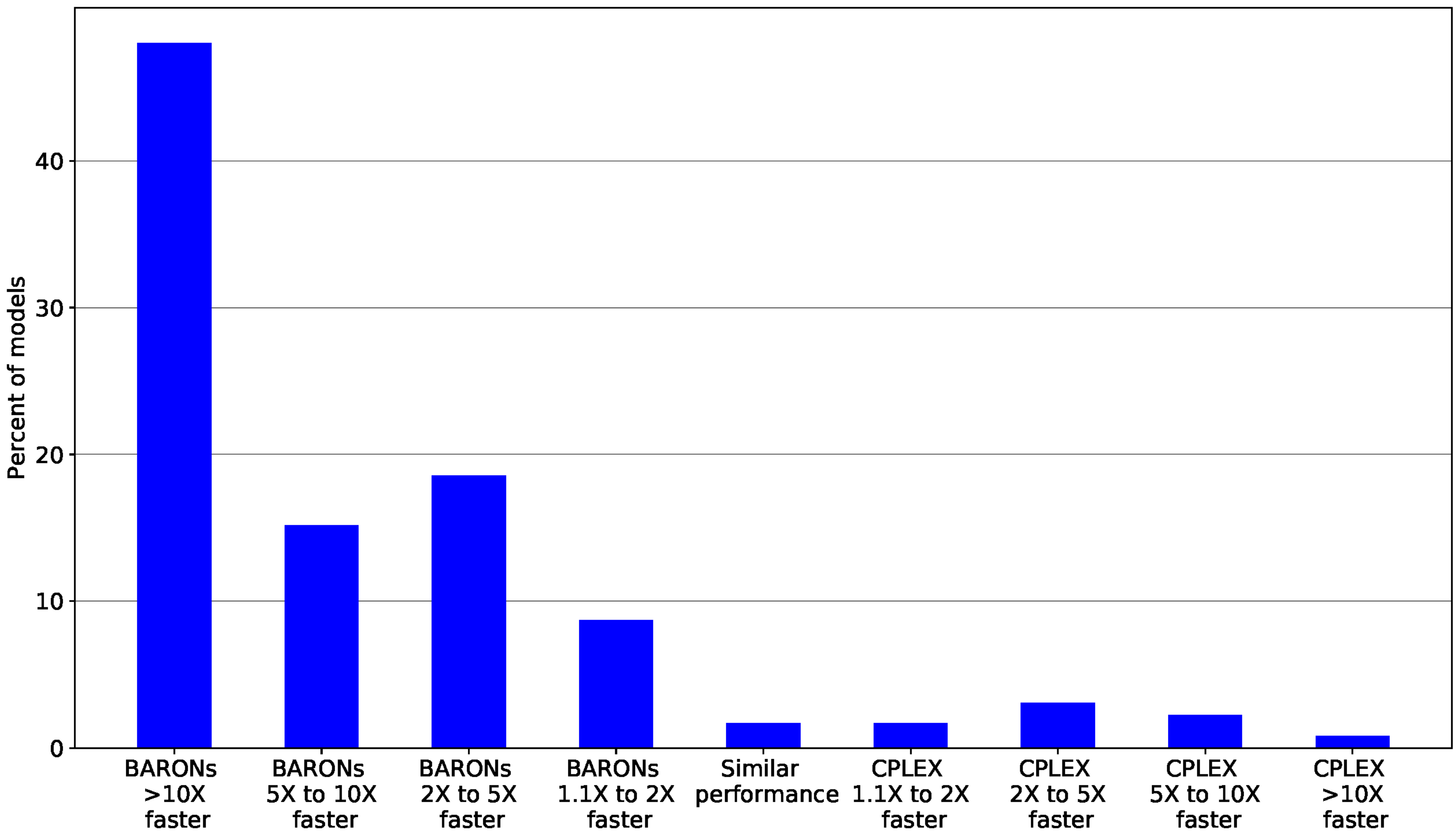


COMPARISON WITH OTHER SOLVERS

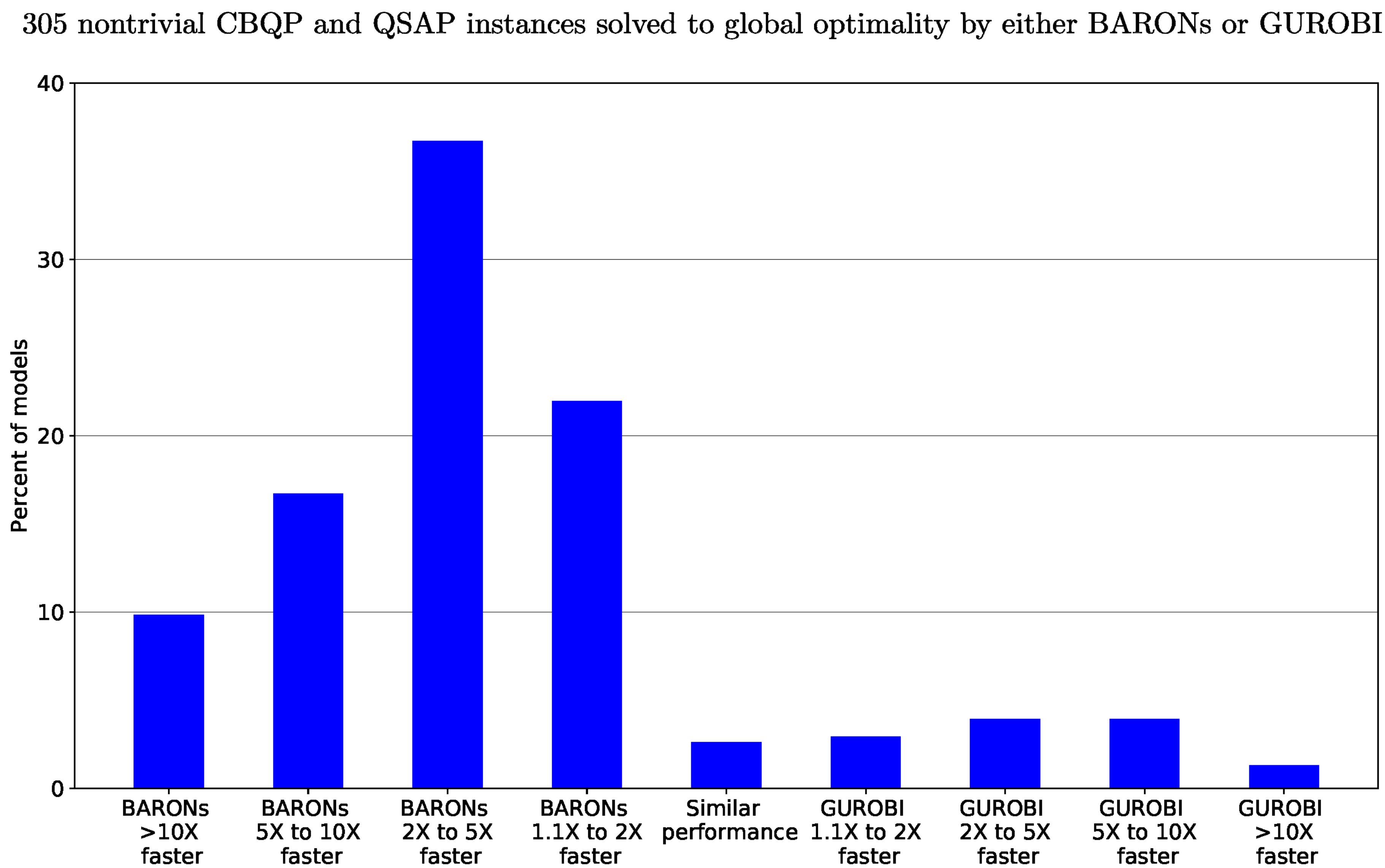


COMPARISON WITH CPLEX

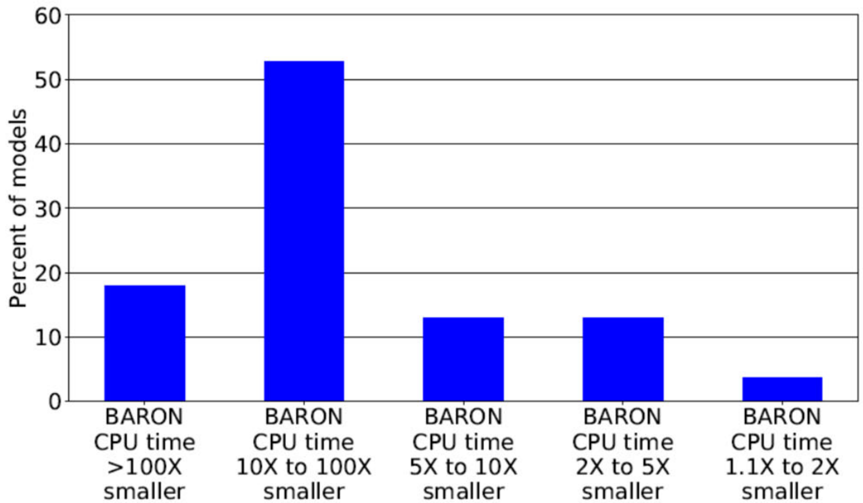
356 nontrivial CBQP and QSAP instances solved to global optimality by either BARONs or CPLEX



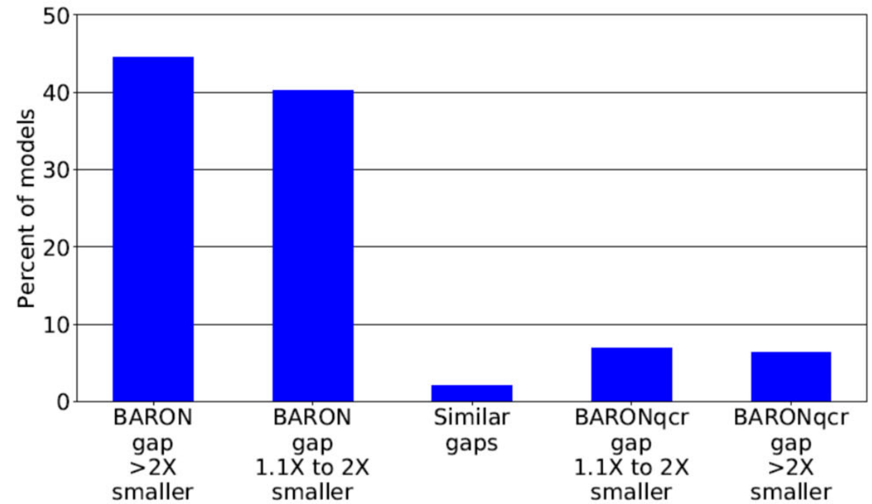
COMPARISON WITH GUROBI



COMPARISON TO QCR



(a) CPU times (442 nontrivial instances).



(b) Relative gaps (537 nontrivial instances).

- **Quadratic convex reformulations for binary quadratic programs (Billionnet et al., 2009, 2013)**
  - Tighter than eigenvalue relaxations at the root node
  - Much slower to converge

SPECTRAL RELAXATIONS

- Despite their simplicity, these relaxations provide **tight bounds for many problems**
- Constructed **in the space of original problem variables**, they are **very inexpensive to solve**
- **Equivalent to some particular SDPs**
- Lead to **very significant improvements** in the performance of branch-and-bound algorithms
- Useful for **dense** problems