Combinatorial Algorithm for Quadratic Programs with Laplacian Structure

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Abstract

An algorithm is presented that uses a mostly combinatorial approach to solve a family of convex quadratic programs over box constraints. It is proved that for convex programs with the required structure, the algorithm converges in a finite number of iterations. Moreover, each iteration requires, at most, one function evaluation. On synthetic problems with thousands of variables, our implementation determines the optimal solution in seconds.

1 Context and previous work.

Quadratic programming problems play a unique role in optimization theory [38]. The general quadratic problem consists of a quadratic objective function and a set of linear inequality constraints. This paper will focus on a quadratic programming problem with n variables subject to a set of box constraints:

$$\min\{\frac{1}{2}x^tQx + c^tx \mid l \leq x \leq u\}, \tag{1}$$

where x is a vector of decision variables, $Q \in R^{n\times n}$ is a symmetric matrix of quadratic costs (not necessarily positive definite), $c \in R^n$ is a column vector of linear costs, and $l \in R^n$ and $u \in R^n$ are the vectors of lower and upper bounds, respectively [3, 7]. If matrix Q is positive definite or positive semidefinite, then (1) becomes a convex programming problem, [6, 20] making the local optimum equivalent to the global optimum. Therefore, (1) can be solved in polynomial time by using a wide array of optimization algorithms [2, 6, 7, 8, 12, 13, 17, 20, 22, 24, 27, 28, 29, 32, 38]. For indefinite Q, (1) is NP-hard [3, 7, 21].

Quadratic programming problems with box constraints arise frequently in both applications [1, 4, 19, 23, 26, 30, 31, 33] and mathematical practice

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[5, 6, 7, 9, 11, 13, 14, 17, 18, 22, 24, 28, 29, 34, 35]. Quadratic programming problems are usually solved with one of three approaches: active sets, conjugate gradients, or interior points [7, 11, 13, 28, 31, 38]. Active set approaches usually terminate in a finite number of iterations [3, 7, 8, 28, 29] but at each step they modify only two variables imposing a lower bound on the number of iterations required for convergence. Thus, the number of iterations can be large [28, 29]. Moreover, they must avoid cycling, especially in the case of degenerate problems. The gradient-related approaches typically converge fast, [25] but require a number of function and gradient evaluations at each step [7, 28, 31]. The interior-point methods are generally very efficient and have good convergence bounds [12, 15, 16, 36, 39] but must take care, at termination, to jump to a boundary as all iterations were interior to the feasible region and approximated by floating point numbers.

In contrast, the algorithm presented here only applies to convex problems with a special structure, but in those cases, it suffers from none on the previously mentioned shortcomings. It is combinatorial in nature and can be implemented over the rationals, eliminating any floating point inaccuracies. It converges in a finite number of iterations, typically much smaller than active set methods, because multiple variables can be modified per iterations. Finally, the iterations do not require any function evaluation.

1.1 Motivational example.

Before generalizing, we illustrate the type of problems under consideration and the solution technique. Consider a data set of stock prices with the lowest and highest values of the day read over a period of $N+1$ days: $[l_1, h_1], [l_2, h_2], \ldots, [l_{N+1}, h_{N+1}]$. We wish to find most representative prices as well as the "best" mean and variance to summarize the data. We will define "best" as the solution to

$$\min \left\{ \Pi_{i=1}^{i=N} \frac{1}{\sqrt{2\pi}\sigma} e^{\frac{-(p_{i+1}-p_i-\nu)^2}{\sigma^2}} \mid p_i \in [l_i, h_i] \right\}. \tag{2}$$

We do not care about the optimal value, but only about the optimal solution. By taking the log, and considering each box constraint, we can transform (2) into

$$\min \left\{ \rho(x, \nu, \sigma) := N \log \sigma - \frac{\sum_i (x_i - \nu)^2}{2\sigma^2} \mid x_i \in [a_i, b_i] \right\} \tag{3}$$

where

$$\begin{aligned} a_i &= l_{i+1} - h_i, \\ b_i &= h_{i+1} - l_i. \end{aligned}$$

Under this form (3), it is clear that the problem is ill-posed if the intersection of the box constraints is non-empty. For then, we can take $x_i = \nu$ and $\sigma \to 0$ to drive the program to $-\infty$. We will therefore make an important assumption throughout the paper: This is equivalent to restricting the original form (2) not to have a solution with exponential increase.

Assumption 1. *The box constraints have empty intersection or,*

$$\cap_i \, [a_i, b_i] = \emptyset. \tag{4}$$

We note that the problem is not convex. To see this, let us consider a small-dimensional case.

$$\frac{(x_1 - \nu)^2}{2\,\sigma^2} + \frac{(x_2 - \nu)^2}{2\,\sigma^2} + 2\log\sigma$$

with gradient

$$\left[\frac{\mathrm{x_1}-\nu}{\sigma^2} \quad \frac{\mathrm{x_2}-\nu}{\sigma^2} \quad -\frac{\mathrm{x_2}-\nu}{\sigma^2} - \frac{\mathrm{x_1}-\nu}{\sigma^2} \quad -\frac{(\mathrm{x_2}-\nu)^2}{\sigma^3} - \frac{(\mathrm{x_1}-\nu)^2}{\sigma^3} + \frac{2}{\sigma}\right]^t$$

and Hessian

$$\begin{bmatrix} \frac{1}{\sigma^2} & 0 & -\frac{1}{\sigma^2} & -\frac{2\,(\mathrm{x_1}-\nu)}{\sigma^3} \\ 0 & \frac{1}{\sigma^2} & -\frac{1}{\sigma^2} & -\frac{2\,(\mathrm{x_2}-\nu)}{\sigma^3} \\ -\frac{1}{\sigma^2} & -\frac{1}{\sigma^2} & \frac{2}{\sigma^2} & \frac{2\,(\mathrm{x_2}-\nu)}{\sigma^3} + \frac{2\,(\mathrm{x_1}-\nu)}{\sigma^3} \\ -\frac{2\,(\mathrm{x_1}-\nu)}{\sigma^3} & -\frac{2\,(\mathrm{x_2}-\nu)}{\sigma^3} & \frac{2\,(\mathrm{x_2}-\nu)}{\sigma^3} + \frac{2\,(\mathrm{x_1}-\nu)}{\sigma^3} & \frac{3\,(\mathrm{x_2}-\nu)^2}{\sigma^4} + \frac{3\,(\mathrm{x_1}-\nu)^2}{\sigma^4} - \frac{2}{\sigma^2} \end{bmatrix}$$

The 3×3 upper-left sub-block has eigenvalues $\{\frac{1}{\sigma^2}, \frac{3}{\sigma^2}, 0\}$, and is therefore positive semi-definite. The bottom-right block can be positive or negative in general, indicating an indefinite Hessian.

1.2 Optimality conditions.

Let us consider necessary conditions for optimal solutions.

Theorem 1. *If x^*, ν^*, σ^* are optimal for* (3)*, then*

1. *If $x_i^* = a_i$ then $x_i^* \geq \nu^*$.*
2. *If $x_i^* = b_i$ then $x_i^* \leq \nu^*$.*
3. *If $x_i^* \in (a_i, b_i)$ then $x_i^* = \nu^*$.*
4. *$\nu^* = \frac{1}{N} \sum_{i=1}^N x_i^*$.*
5. *$(\sigma^*)^2 = \frac{1}{N} \sum_{i=1}^N (x_i^* - \nu^*)^2$*

Proof. The proof follows from the fact that the feasible region is convex. The tangent cone of feasible directions, T, is generated by

$$d_i = [0, \ldots, 0, \alpha_i, 0, \ldots, 0]$$

where

- $\alpha_i > 0$ for all i where $x_i^* = a_i$,
- $\alpha_i < 0$ for all i where $x_i^* = b_i$,
- α_i is free for all i where $x_i^* \in (a_i, b_i)$, $i = N+1$ and $i = N+2$.

Since x^*, ν^*, σ^* is optimal,

$$\nabla\rho(x^*, \nu^*, \sigma^*)^t d \geq 0 \quad , \forall d \in T.$$

By considering each generator, d_i,

$$\nabla\rho^t d_i = \left[\frac{x_1 - \nu}{\sigma^2}, \ldots, \frac{x_N - \nu}{\sigma^2}, \ldots, -\frac{\sum(x_i - \nu)}{\sigma^2}, \frac{N}{\sigma} - \frac{\sum(x_i - \nu)^2}{\sigma^3}\right] d_i \geq 0.$$

The result follows. □

We can now transform the problem by constraining ν and σ to obtain

$$\min\left\{N\log\sigma - \frac{\sum_i (x_i - \nu)^2}{2\sigma^2} \mid x_i \in [a_i, b_i], \nu = \frac{\sum_i x_i}{N}, \sigma^2 = \frac{\sum_(x_i - \nu)^2}{N}\right\}.$$

After substitution of ν and σ, we obtain

$$\min\left\{\frac{N}{2} + \frac{N}{2}\log\left(\frac{N-1}{N^2}\sum_i x_i^2 - \frac{1}{N^2}\sum_i\sum_{j\neq j} x_i x_j\right)^{\frac{1}{2}} \mid x_i \in [a_i, b_i]\right\}.$$

Since log and $\sqrt{}$ are monotone increasing we discard them as well as the constants to obtain our final formulation

$$\min\left\{\bar{\rho}(x) = (N-1)\sum_i x_i^2 - \sum_i\sum_{j\neq i} x_i x_j \mid x_i \in [a_i, b_i]\right\}. \tag{5}$$

2 Laplacian quadratic program.

Problem (5) does not have the same optimal value as (2). In fact, we have transformed a seemingly non-convex problem into a convex one. Both problems share the same optimal solution for the x_i. From these, we can

retrieve the ν and σ of the original problem. In passing, we note that problem (5) is a constrained least-squares problem:

$$\min\{\frac{1}{2}\|H^{\frac{1}{2}}x\|^2 \mid x_i \in [a_i, b_i]\} \tag{6}$$

where

$$H = \begin{bmatrix} (N-1) & -1 & -1 & \dots & -1 \\ -1 & (N-1) & -1 & \dots & -1 \\ -1 & -1 & (N-1) & \dots & -1 \\ \vdots & & & \ddots & \\ -1 & -1 & -1 & \dots & (N-1) \end{bmatrix}. \tag{7}$$

Theorem 2. *The optimal solution for problem* (5) *is unique and is an optimal solution for problem* (2).

Proof. First, we note that problem (5) is convex. The hessian $\nabla^2\bar{\rho}(x) = 2H$, where H is defined at (7). The Hessian has eigenvalues 0 and $2N$, the latter with multiplicity $N-1$. Therefore, the necessary conditions for optimality are sufficient. The gradient is

$$\nabla\bar{\rho}(x) = \left[2(N-1)x_1 - 2\sum_{j\neq 1} x_j, \dots, 2(N-1)x_N - 2\sum_{j\neq N} x_j\right]^t.$$

An optimal x^* satisfies exactly the same conditions as in Theorem 1, that is

- If $x_i^* = a_i$ then $x_i^* \geq \frac{\sum_i x_i^*}{N}$.
- If $x_i^* = b_i$ then $x_i^* \leq \frac{\sum_i x_i^*}{N}$.
- If $x_i^* \in (a_i, b_i)$ then $x_i^* = \frac{\sum_i x_i^*}{N}$.

Therefore, an optimal solution for (5) is optimal for (2). It remains to show uniqueness.

If there were multiple optimal solutions, they would be along the eigenspace corresponding to the zero eigenvector of the Hessian. This space has basis

$$v = [1, 1, 1, \dots, 1]^t.$$

If a move along this space is feasible, it means that each component of x^* is strictly inside the feasible region, and they are all equal to each other and equal to ν, which is precluded by Assumption 1. □

2.1 A combinatorial algorithm.

The key observation to motivate the algorithm is to recognize the Hessian of (5) as the Laplacian of the complete graph K_N. In general, the Laplacian of a graph is

$$x^t(D - A)x,$$

where D is a diagonal matrix of the degrees. In the case of K_N, it is $(N-1)I$. Finally, A is the adjacency matrix where $A_{i,j} = 1$ if and only if there is an edge between i and j (all pairs in the case of K_N).

With this observation, we can interpret Problem (5) (or, more appropriately, Problem (6)) as the problem of partitioning the graph under uncertainty of the node weights. Each box constraint is an indication of the possible weight of the node. We will therefore adapt well-known approaches to this situation.

The general idea is the following. Create a vector of all boundary values $[a_1, b_1, a_2, b_2, \ldots, a_N, b_N]$, then sort uniquely. We call these values the potentials. Choose an estimate $\bar{\nu}$ from these potentials, possibly the value closest to the median of all mid-points of the box constraints, but any measure of centrality would work. Assign to each x_i the value in $[a_i, b_i]$ closest to $\bar{\nu}$. This will be the lower bound if $\bar{\nu}$ is smaller, or the upper bound if $\bar{\nu}$ is larger, or $\bar{\nu}$ if it falls within the bounds. Then, as long as the objective value improves, move $\bar{\nu}$ to the next boundary value and repeat. In detail, Algorithm 1.

Data: The box: $r = ((a_1, b_1), (a_2, b_2), \ldots, (a_N, b_N))$.
Result: The optimal x^*.
$p = sort(flatten(r))$ /* The list of potentials. */;
$i = \lfloor \frac{len(p)}{2} \rfloor$ /* Index of initial estimate. */;
$s = False$;
repeat
  $\bar{\nu} = p[i]$ /* Next estimate. */ ;
  Compute x as Equation (8) ;
  $\nu = \frac{1}{N} \sum_i x_i$ /* True mean. */;
  if $s = False$ **then**
    $s = sign(\nu - \bar{\nu})$ /* Direction of movement. */;
  end
  $i = i + s$ /* Index of adjacent boundary value. */;
until $s = 0 \vee s \neq sgn(\nu - \bar{\nu})$;
Compute d as Equation (9);
$\alpha = \frac{N(\bar{\nu} - \nu)}{N - |I^+|}$;
$x^* = x + \alpha d$;

Algorithm 1: Solver for Problem (6)

The details and the proof of correctness will follow after some prelim-

inaries. First, given an estimate $\bar{\nu} \in [\min_i\{a_i\}, \max_i\{b_i\}]$, we define a feasible solution $\bar{x}$ as

$$\bar{x}_i := \begin{cases} a_i & \bar{\nu} \leq a_i, \\ b_i & b_i \leq \bar{\nu}, \\ \bar{\nu} & \bar{\nu} \in (a_i, b_i). \end{cases} \tag{8}$$

Intuitively, we set the solution to be as close to the estimate $\bar{\nu}$ as possible. We also define the true mean $\nu := \frac{\sum_i x_i}{N}$ and a feasible direction d as

$$d_i := \begin{cases} 1 & \bar{\nu} < \nu \bigwedge a_i \leq \bar{\nu} = x_i < b_i, \\ -1 & \nu < \bar{\nu} \bigwedge a_i < x_i = \bar{\nu} \leq b_i, \\ 0 & \text{otherwise.} \end{cases} \tag{9}$$

Note that d is either composed of $\{0, 1\}$ or $\{-1, 0\}$. Let us name the index sets $I^+ := \{i \mid d_i = 1\}$ and $I^- := \{i \mid d_i = -1\}$; note that they are disjoint. We are now equipped to show decrease of the objective function if we move in the direction d.

Theorem 3. *Given an estimate $\bar{\nu}$, a feasible solution x, a true mean ν and a direction of movement d defined as above, then, if $\bar{\nu} \neq \nu$,*

$$\rho(x + \alpha d) < \rho(x)$$

for α sufficiently small.

Proof. Since ρ is quadratic, decrease is assured if $\nabla\rho(x)^t d < 0$. Let us consider the case $\bar{\nu} < \nu$.

$$\begin{aligned} \nabla\rho(x)^t d &= \sum_i d_i[(N-1)x_i - \sum_{j \neq i} x_j] \\ &= \sum_{i \in I^+} [(N-1)x_i - \sum_{j \neq i} x_j] \\ &= \sum_{i \in I^+} [Nx_i - \sum_j x_j] \\ &= \sum_{i \in I^+} [Nx_i - N\nu] \\ &= N \sum_{i \in I^+} [x_i - \nu] \\ &= N \sum_{i \in I^+} [\bar{\nu} - \nu] \\ &< 0 \end{aligned}$$

The case $\nu < \bar{\nu}$ is symmetric with the signs reversed. □

Theorem 3 allows us to increase the estimate $\bar{\nu}$ by jumping from one box boundary value to the next, usually modifying multiple components of the feasible solution x at each step. We note that this differs from the behavior of active sets methods which will only modify two components at each step, the so-called entering and leaving variables. This is also different from gradient projection type methods which require multiple function and gradient evaluations at each step. We require only the computation of the estimate $\bar{\nu}$, which is a linear time computation. Moreover, our approach is immune to any degeneracy of the problem. In fact, the more degenerate the problem, the more variables will be updated at each step, reducing the number of steps. The termination criteria will depend on the final position of the true mean with respect to the boundary values.

Theorem 4. *The estimate $\bar{\nu}$ either increases or decreases monotonically at each step until the true mean ν lies exactly on a boundary or between two adjacent boundary values. In the former case, the current iterate is optimal. In the latter case, the final step to the optimal solution is given by*

$$x^* = x + \alpha d, \text{ where } \alpha = \frac{N(\bar{\nu} - \nu)}{N - |I^+|} \tag{10}$$

Proof. First note that, if $\bar{\nu} = \nu$ the current iterate is optimal by Theorem 2.

Consider the case $\bar{\nu} < \nu$; the other case is similar. Then, by the definition of d (9), the components of x that are modified are all modified by increasing. The next estimate $\bar{\nu}$ is therefore the adjacent and larger boundary value and the true mean increased. If this true mean is larger than the current estimate, the argument is repeated. If not, then it lies between the last two estimates.

Note that given a direction d, then $f(\alpha) = \rho(x + \alpha d)$ is quadratic in α with minimizer at

$$-\frac{d^t H x}{d^t H d} = -\frac{N(\bar{\nu} - \nu)}{N - |I^+|}.$$

Therefore, the components of the solution that have changed have done so by

$$x_i^+ = x_i - \frac{N(\bar{\nu} - \nu)}{N - |I^+|} d_i = \bar{\nu} - \frac{N(\bar{\nu} - \nu)}{N - |I^+|}$$

while the mean has changed by

$$\nu^+ = \frac{1}{N} \sum_i x_i^+ = \frac{1}{N} \left[\sum_i x_i + \sum_{i \in I^+} -\frac{N(\bar{\nu} - \nu)}{N - |I^+|} \right] = \nu - \frac{|I^+|(\bar{\nu} - \nu)}{N - |I^+|}$$

It remains to show that the components that have changed are now all equal to the mean.

$$\begin{aligned}\nu^+ &= \nu - \frac{|I^+|(\bar{\nu} - \nu)}{N - |I^+|} \\ &= \bar{\nu} - \bar{\nu} + \nu - \frac{|I^+|(\bar{\nu} - \nu)}{N - |I^+|} \\ &= \bar{\nu} - \frac{(N - |I^+|)(\bar{\nu} - \nu)}{N - |I^+|} - \frac{|I^+|(\bar{\nu} - \nu)}{N - |I^+|} \\ &= \bar{\nu} - \frac{N(\bar{\nu} - \nu)}{N - |I^+|}.\end{aligned}$$

The last step therefore reaches the optimal solution. □

We are now equipped to show that the algorithm will terminate in a small number of iterations.

Theorem 5. *Algorithm 1 solves Problem* (5) *in a finite number of iterations and the time complexity is* $O(N^2)$.

Proof. The algorithm terminates because, at each iteration, the estimate $\bar{\nu}$ either increases or decreases monotonically from one boundary value to the next. At most, the number of iterations is the number of boundary values, therefore, N. The loop terminates because either $\nu = \bar{\nu}$ or the mean ν lies between two boundary values. In the former case, the solution is optimal by Theorem 2. In the latter case, the final step computation is the optimal by Theorem 4. At each iteration, the dominant cost is the computation of the mean, hence linear in N, therefore the total cost is bounded by N^2. □

2.2 Numerical experiment.

To validate the algorithm we ran it on synthetic data. At each trial, the ranges were generated randomly from a uniform distribution. We ran trials of increasing sizes, repeating multiple times and averaging the number of iterations. The experimental code is available online at `github.com/sgkruk/Laplacian-QP`. The complete experiment runs in a few seconds and is displayed in Table 1.

3 Conclusions and future work.

The original motivation for the work is a non-convex non-linear stock tracking problem, usually handled by classical continuous techniques. After a sequence of transformations, we obtained a convex quadratic program where

Table 1: Number of variables and average number of iterations.

Dimension	Iterations
10	1
20	3
30	3
50	5
100	10
200	21
300	31
500	54
1000	108
5000	513
10000	1047

the Hessian is recognized as the Laplacian of a graph, suggesting a combinatorial solution technique. The resulting interpretation of the problem is that of bi-partitioning under uncertainty of the node weights. The presented algorithm is combinatorial and theoretically more efficient than a general purpose quadratic algorithm, whether active set, gradient-descent, or interior-point based. It terminates in a finite number of iterations, a number much smaller than active sets. It requires no function evaluation, as gradient-based approaches do. It is immune to degeneracy and our implementation is rational-based therefore not subject to floating point inaccuracies. We are current extending this approach to the solution of more general quadratic programs.

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