Learning to Branch:
New Results for the Quadratic Assignment Problem

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slides + git

bit.ly/kurt-qap

Key Points

Branching is a primary performance driver for branch-and-bound algorithms for the Quadratic Assignment Problem (QAP).

Branching rules obtained by learning-to-rank methods can outperform traditional hard-coded rules.

This approach can likely be used for most QAP bounds, and for problems beyond QAP.

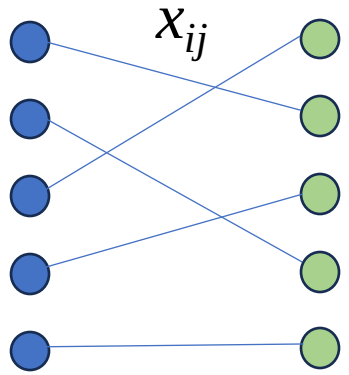
Linear Assignment Problems (LAP)

$$\min \sum_{i,j}^{n} c_{ij} x_{ij}$$

$$\sum_{i}^{n} x_{ij} = 1, \quad j = 1..n$$

$$\sum_{j}^{n} x_{ij} = 1, \quad i = 1..n$$

$$x_{ij} \in \{0, 1\} \qquad X \in \Pi$$



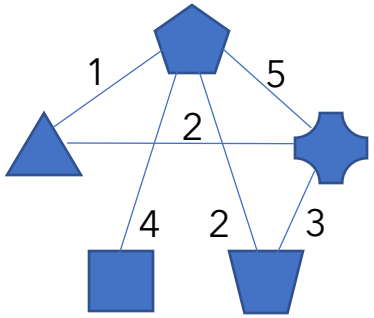
AKA minimum cost weighted bipartite matching

Birkhoff 1946: The permutation matrices constitute the extreme points of the set of doubly stochastic matrices ⟶ x integrality can be relaxed ⟶ LAP is easy

Quadratic Assignment Problem (QAP)

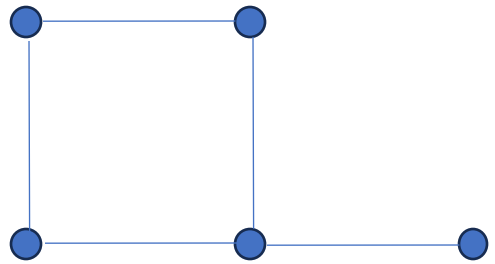
$$\min_{X \in \Pi} \sum_{i,j,k,l}^{n} a_{ij} b_{ij} x_{ij} x_{kl} + \sum_{i,j}^{n} c_{ij} x_{ij}$$

flows (A)



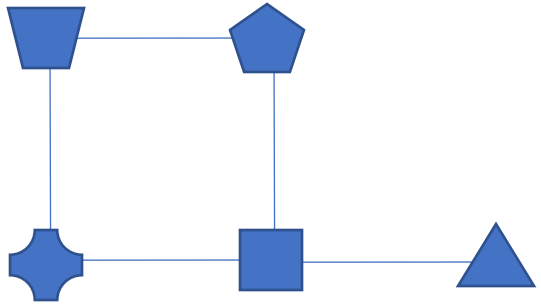
$$\begin{bmatrix} 0 & 5 & 2 & 4 & 1 \\ 5 & 0 & 3 & 0 & 2 \\ 2 & 3 & 0 & 0 & 0 \\ 4 & 0 & 0 & 0 & 0 \\ 1 & 2 & 0 & 0 & 0 \end{bmatrix}$$

distances (B)



$$\begin{bmatrix} 0 & 1 & 2 & 2 & 3 \\ 1 & 0 & 2 & 1 & 2 \\ 2 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 \\ 1 & 2 & 0 & 0 & 0 \end{bmatrix}$$

assignment (X)



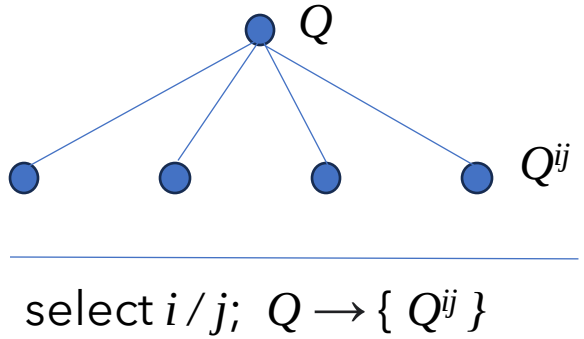
$$\begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

Divide and Conquer using Partial Assignments

Let $Q = (A, B, C)$ be a QAP of size n.

Assigning $i \rightarrow j$ yields a QAP Q^{ij} of size n-1:

$$
\begin{aligned}
Q^{ij} &= (A^{ij}, B^{ij}, C^{ij}, d^{ij}) \\
A^{ij} &= A_{(ii)} \\
B^{ij} &= B_{(jj)} \\
C^{ij} &= C_{(ij)} + 2\hat{a}_i \hat{b}_j \\
d^{ij} &= a_{ii} b_{jj} + c_{ij}
\end{aligned}
$$



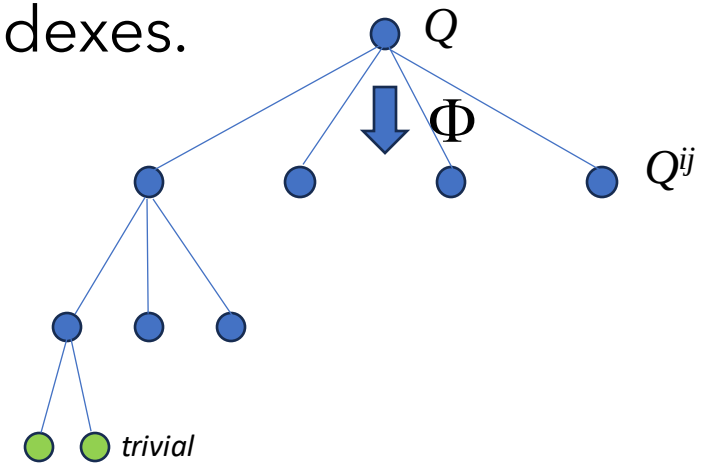
where

$M_{(ij)}$ = M with row i and column j removed

$\hat{a}_i$ = row i of A with ith element removed

Solving QAP using Enumeration Trees

Let $I = I_R \cup I_C$ be the set of row and column indexes.



Selecting $i \in I$ is called *branching*.

$\Phi(Y) \rightarrow i$ is a *branching method*.

Repeatedly applying Φ generates a tree of QAPs, with trivial subproblems at the leaves.

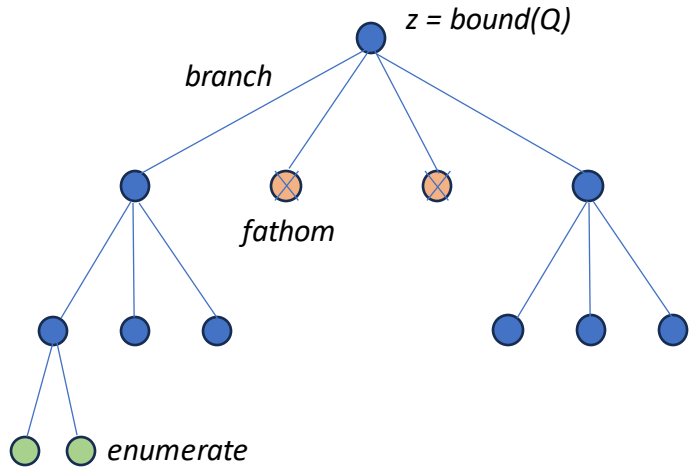
The size of the tree is exponential in n.

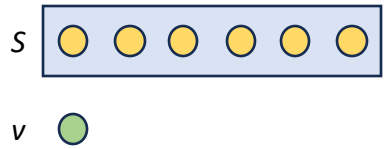
Branch and Bound: Trimmed Enumeration Trees

```
def branch_and_bound(P):
  v = initial_solution(P)
  S = {P}

  while not empty(S):
    Q = take(S)
    if easy(Q):
      v = enumerate(Q, v)
    else:
      z, Y = bound(Q) # Y = branching context
      if z <= v: # no fathom
        S += branch(Q, Y)

  return v
```





Branch and Bound: Four Things Matter

Thing	Aspiration	Metric
Bound Quality	Fathom as often as possible	(z – w) / w
Bound Speed	Calculate as fast as possible	cpu time
Branching Quality	Make future nodes as easy as possible	??
Branching Speed	Create new nodes as fast as possible	cpu time

Lots of research about this…

…not nearly as much about this

Quadratic Programming Bound: pretty fast, pretty good

Anstreicher, Brixius (2001):

$$\begin{aligned} \text{QPB}: \quad & \min \ \mathbf{vec}(X)^T Q \, \mathbf{vec}(X) + C \bullet X + \langle \lambda(\hat{A}), \lambda(\hat{B}) \rangle_- \\ & \text{s.t.} \ \ Xe = X^T e = e \\ & \qquad X \geq 0, \end{aligned}$$

For easily computed Q, A, B, S, T.

Advantages:

Good quality	Iterative solve → can stop anytime
Can solve fast using LAP	Yields dual matrix U

See also: Recent advances in the solution of quadratic assignment problems - Anstreicher (2003)

QPB vs Gilmore-Lawler (GLB) for nug18 test problem

```
    Total Time: 39.8741 seconds
         Nodes: 265917 / 215368 / 0
    root bound: 1688.79
 fw iterations: 7668323

level    nodes  %fathom %c.elim     time
 0           1  0.0000  0.0000     0.18
 1          18  0.0000  0.0131     1.94
 2         302  0.0033  0.1186     2.34
 3        4245  0.3965  0.3452     3.04
 4       25165  0.6500  0.4911     6.43
 5       62741  0.7630  0.5821    10.53
 6       80792  0.8339  0.6398     9.10
 7       57990  0.8739  0.6806     4.56
 8       25682  0.9014  0.7156     1.41
 9        7202  0.9204  0.7194     0.29
10        1447  0.9109  0.7277     0.05
11         281  0.9253  0.7143     0.01
12          42  0.9048  0.7500     0.00
13           6  0.6667  0.7000     0.00
...
```

```
    Total Time: 244.089 seconds
         Nodes: 34717569 / 25994653 / 5
    root bound: 1554
 fw iterations: 0

level    nodes  %fathom %c.elim     time
 0           1  0.0000  0.0000     0.00
 1          18  0.0000  0.0000     0.00
 2         306  0.0000  0.0000     0.01
 3        4896  0.0071  0.0199     0.08
 4       71465  0.0649  0.1282     0.99
 5      815646  0.2792  0.3498     8.80
 6     4969819  0.5441  0.5546    42.93
 7    12111005  0.7279  0.6882    88.74
 8    11303625  0.8316  0.7669    72.26
 9     4435710  0.8849  0.8073    25.25
10      885601  0.9114  0.8269     4.50
11      108631  0.9232  0.8293     0.50
12        9965  0.9264  0.8147     0.04
13         815  0.9276  0.7932     0.00
...
```

Branching using dual information

Many bounds produce dual matrices U that are useful for branching.

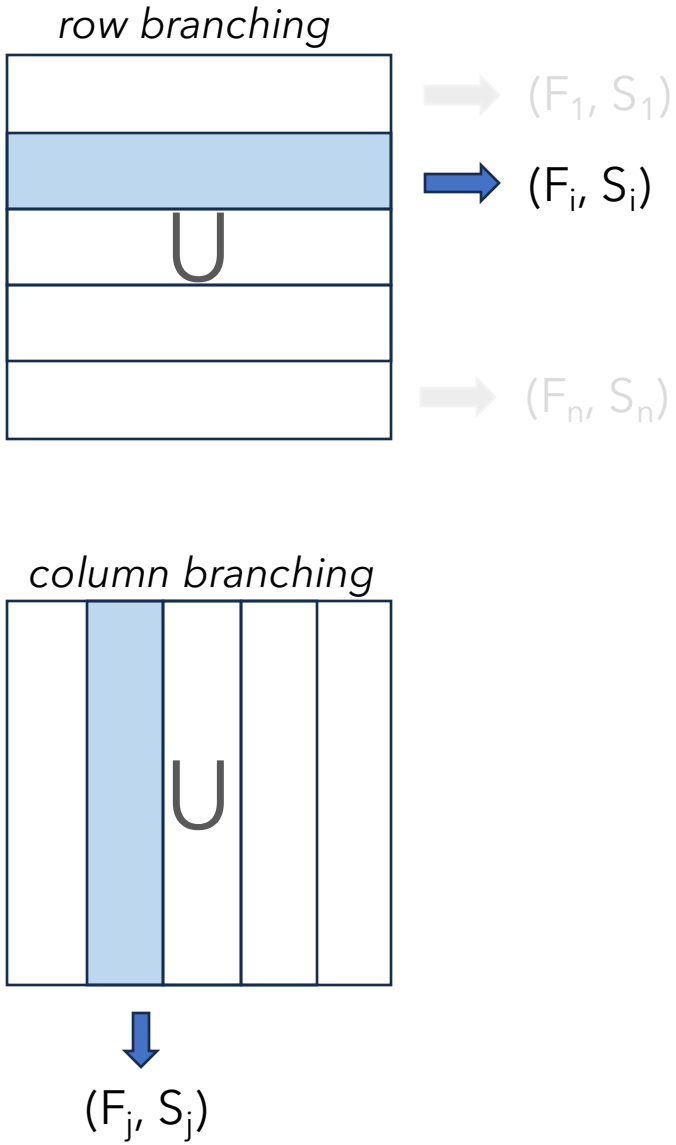
Suppose $u_{ij} \leq bound(Q_{ij})$.

Let's minimize the number of subproblems created, using net bound improvement as a tiebreaker.

$$\Phi(Y) = arg\ lexmin_i\ (f_i, s_i)$$

$$f_{ij}^r = \begin{cases} 1 & \text{if } z_{ij} \geq bound(Q_{ij}) + u_{ij} \\ 0 & \text{otherwise} \end{cases}$$

$$s_{ij}^r = \sum_j u_{ij}$$



Strong branching uses bounds from subproblems

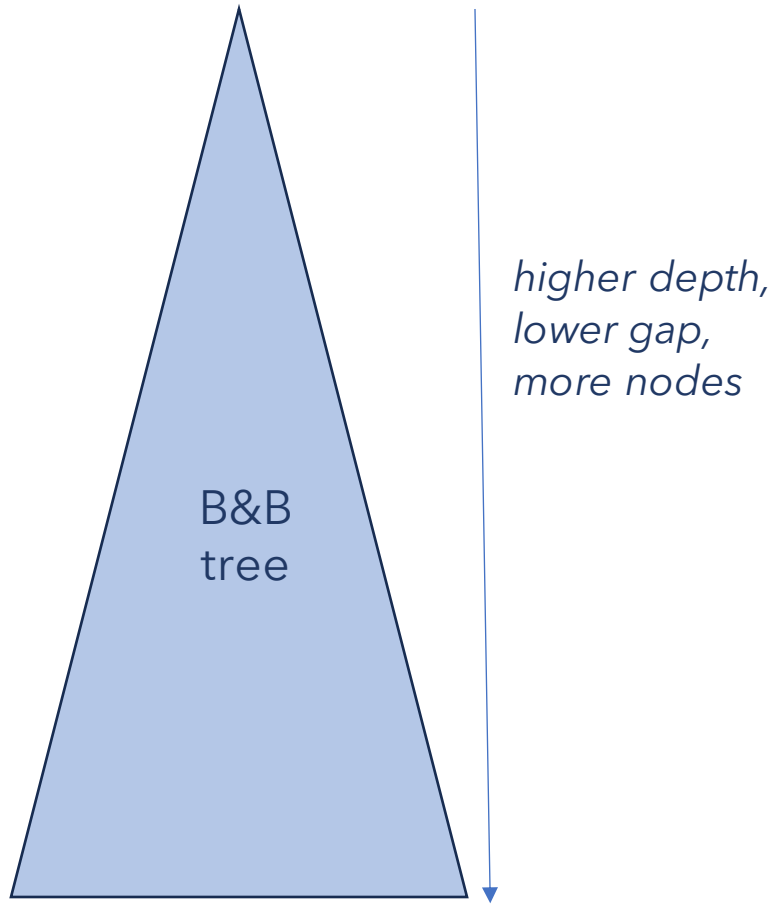
Let $z_{ij} = bound(Q_{ij})$

Strong branching: Φ defined as before, using Z in place of U.

Computational cost is $O(B\ n^2)$ where B is the cost of the bound

Lookahead branching combines strong branching and dual branching:

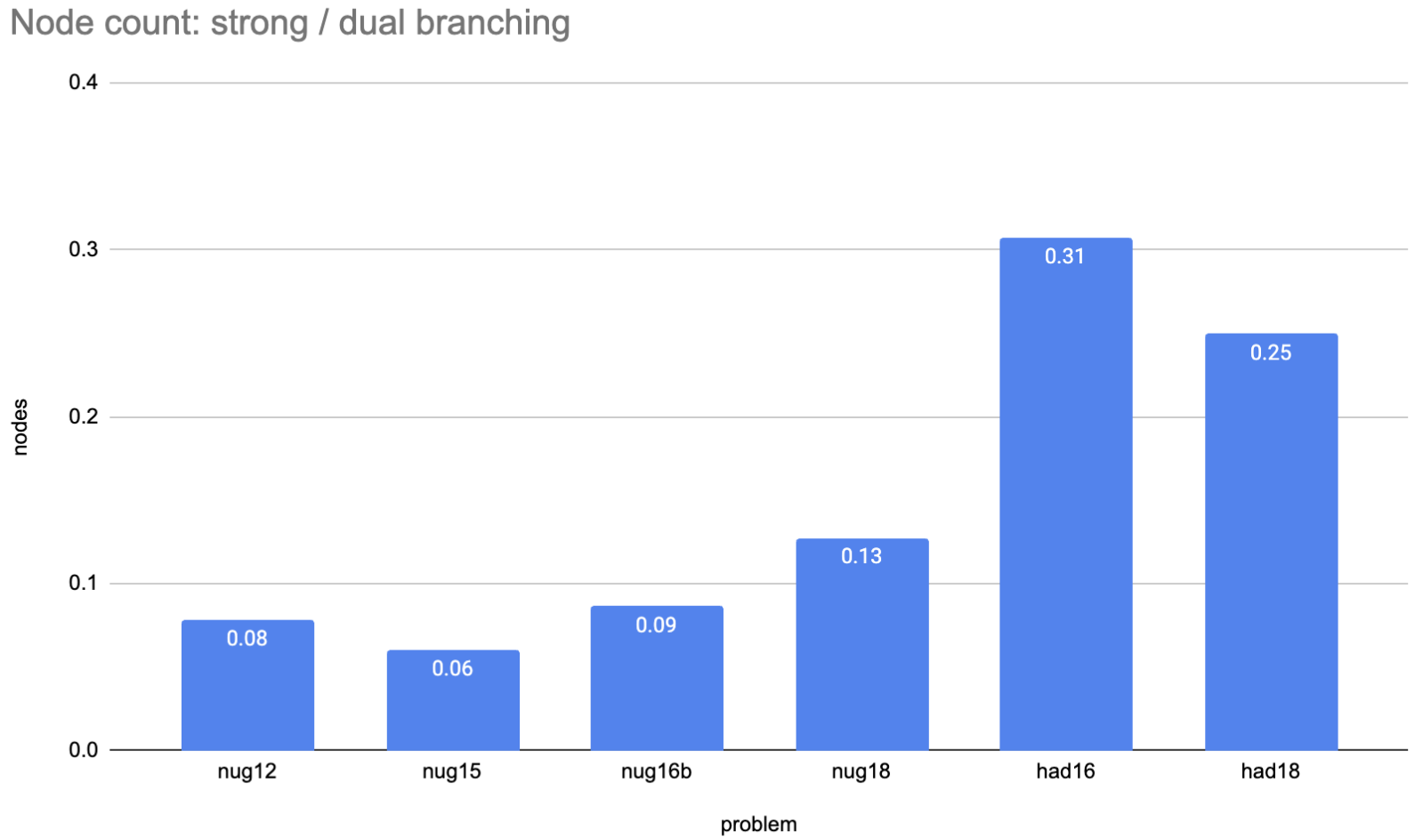
- Z at level $n+1$
- U at level $n+2$ (which comes for free when computing Z)



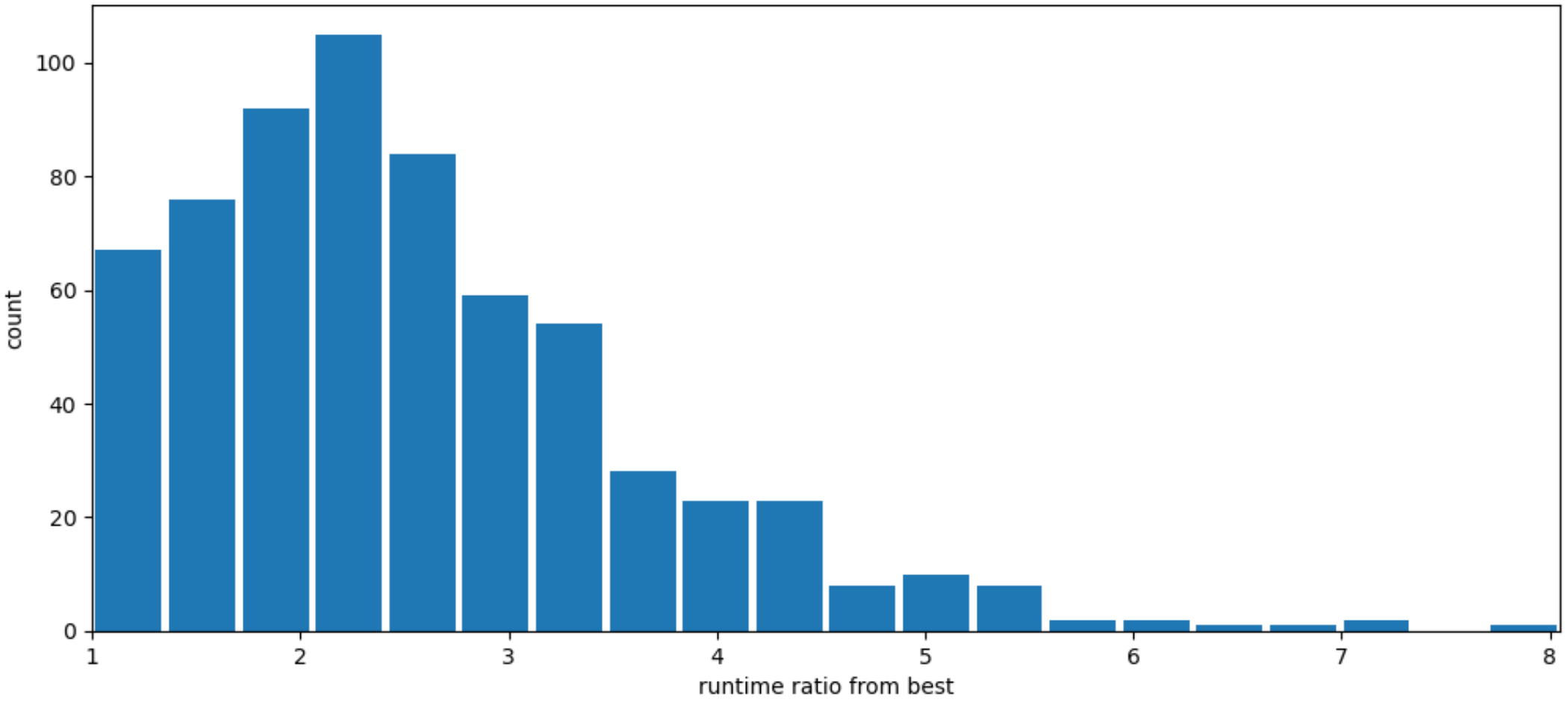
use higher quality, higher cost branching methods selectively

Strong branching reduces tree size

Reduction in nodes from strong branching increases with problem size

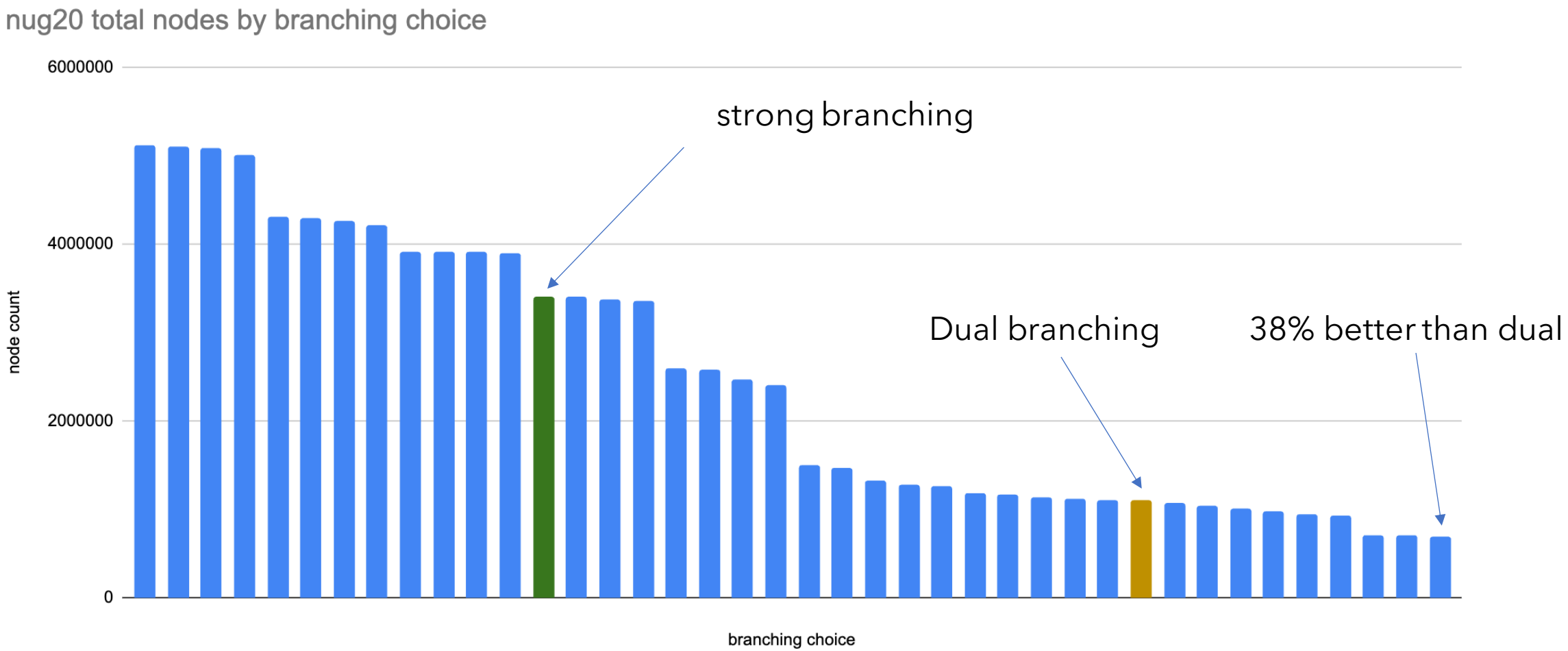


Variance of 650 branching choices at level 4 of nug16b



Variance from a **single** branching choice

Branching matters even more for larger problems



7.5x between best and worst: one branching choice

Finding branching rules is a learning to rank problem

What matters is which branching choice is best:

$$\arg\min_{i \in I} \Phi(Y_i)$$

If choice quality is given by a loss function L:

$$\arg\min_{R(\Phi)} L(\Phi)$$

Minimizing the loss function over the space of ranking models is a **learning-to-rank** problem.

L should involve t_i, the B&B running time given choice i.

Learning-to-rank with Lambdarank

Given q queries each with

- Features F
- Ground truth relevance rank Y

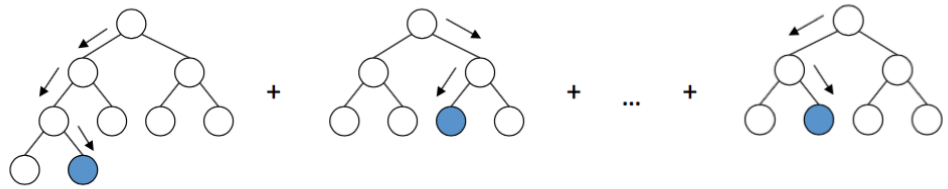
Want estimated relevance score s:

$$\min_{s} \sum_{Y_i > Y_j} \omega(i,j) \log(1 + e^{-\sigma(s_i - s_j)})$$

Lambdarank minimizes this logloss by gradient boosting on (F, Y).

Trained model is a set of if-else decision trees on the features F.

i	s	rank(s)	t
0	0.657	14	157
1	0.631	12	145
2	0.432	3	73
3	0.898	23	267
4	0.123	1	75
..			...
29	0.852	28	311



See:

- "From RankNet to LambdaRank to LambdaMART: An Overview" Burges (2010)
- "The inner workings of the lambdarank objective in LightGBM" Fineis (2021)

Lambda branching: Learning-to-rank in B&B

Create Training Data

Run B&B and log the following:

- `trial, i, X, U, w, z, t`

Prepare Feature Data

```
F = trial | U
Y = t
```

Train Model

```
m = lgb.train(X, y, 'lambdarank')
```

Generate Branching Code

New branching method "lambda"

Offline

bnb

features

lightGBM

Online

bnb

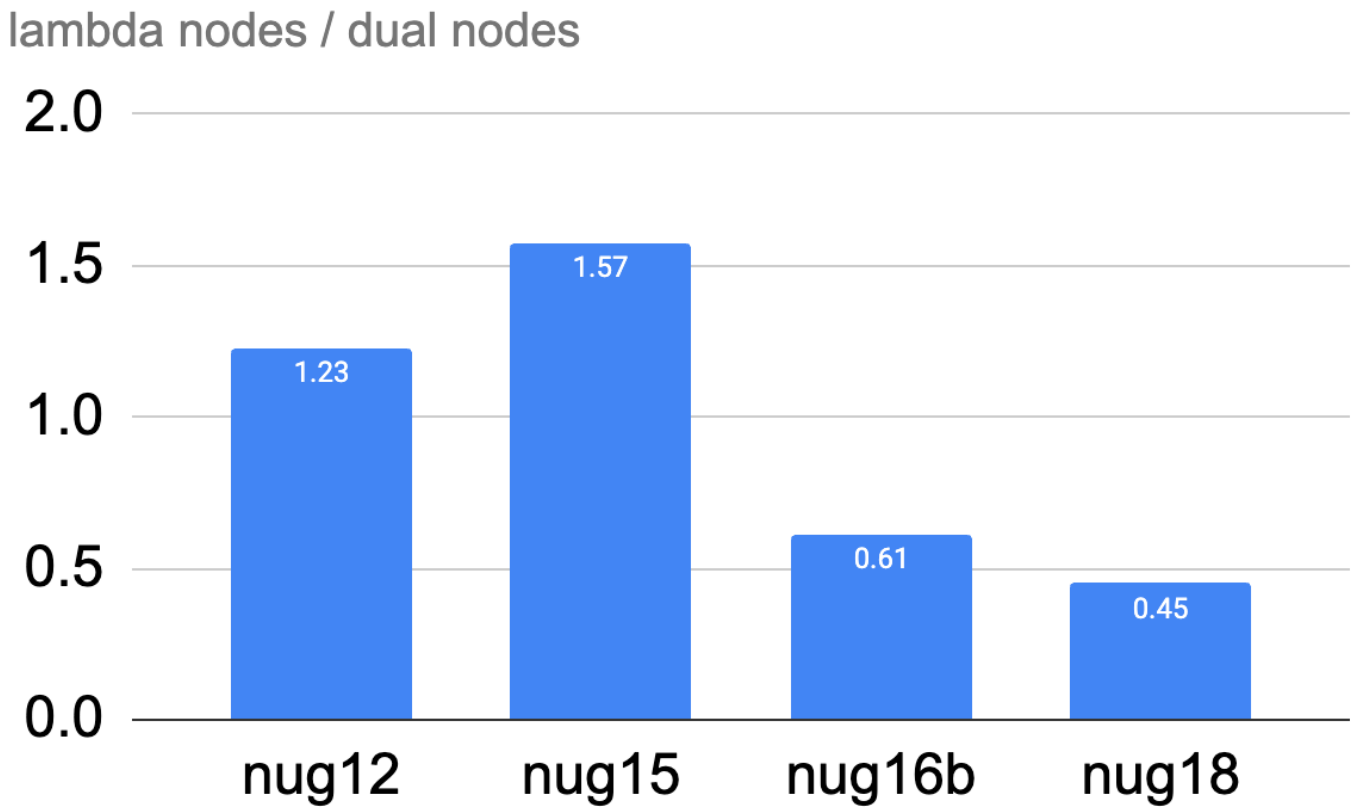
```
void bnb_0(…) {

  if (use_new_branching_method) {
     choice = branch_lgb(…);
  }
}
```

bnb

```
// Generated on 2023-02-24
21:49:18.019726
double boost_0(double * u) {
  if (u[12] <= 0.724678161114384) {
    return 0.7202843678214546;
  }
  else {
    if (u[9] <= 2.137205973102727) {
      if (u[5] <= 0.05828602295712177) {
        return 0.650256793334275;
      }
// ...
```

Lambda compared with dual branching is promising



problem	dual	lambda
nug12	1746	2145
nug15	9338	14705
nug16b	28318	17365
nug18	869707	391055

Next Steps and Extensions

Improve utility for QAP

- Use for strong branching
- Feature engineering: X, (A, B, C), transforms
- Improved tuning and training

Extending usage

- Learn branching strategy selection rules
- Domains outside QAP

In Closing...