Nonnegative/Binary Matrix Factorization with a D-Wave Quantum Annealer

Daniel O'Malley (EES-16), Velimir V. Vesselinov (EES-16)
Boian S. Alexandrov (T-1), Ludmil B. Alexandrov (T-6)
Los Alamos National Laboratory

ISTI D-Wave Rapid Response
April, 27 2017

LA-UR-17-23437

Los Alamos
NATIONAL LABORATORY
EST.1943

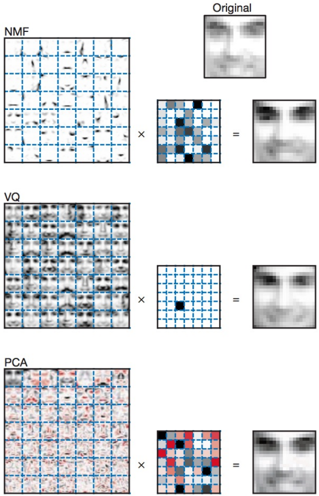
Matrix factorization is a fundamental applied math problem

- SVD: $A = U\Sigma V^*$ where Σ is diagonal, U, V are unitary
- QR: $A = QR$ where Q is orthogonal, R is upper triangular
- LU: $A = LU$ where L is lower triangular and R is upper triangular
- Cholesky: $A = LL^*$ where L is lower triangular
- NMF: $A \approx BC$ where $B_{ij} \geq 0$ and $C_{ij} \geq 0$
- D-Wave NMF: $A \approx BC$ where $B_{ij} \geq 0$ and $C_{ij} \in \{0, 1\}$

Low-rank matrix factorizations

$$\begin{bmatrix} \\ \\ \\ \\ & & & A & & & \\ \\ \\ \\ \end{bmatrix} \approx \begin{bmatrix} \\ \\ \\ \\ & B & \\ \\ \\ \\ \end{bmatrix} \begin{bmatrix} & & & C & & & \end{bmatrix}$$

Unsupervised ML via matrix factorization

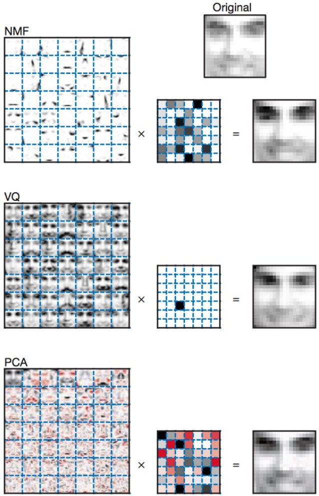


Lee & Seung (Nature, 1999)

$A = BC$

- Each column of A is a vectorized version of an image of a face
- Each row of A corresponds to a particular pixel in the images
- Each column of B is a “feature” that is used to reconstruct the image
- Each row of B corresponds to a particular pixel in the images
- Each column of C corresponds to an image and describes how each feature is present in the image
- Each row of C corresponds to a feature and describes how that feature is present in all the images

Unsupervised ML via matrix factorization on the D-Wave



Lee & Seung (Nature, 1999)

Are some of those features solid black? No

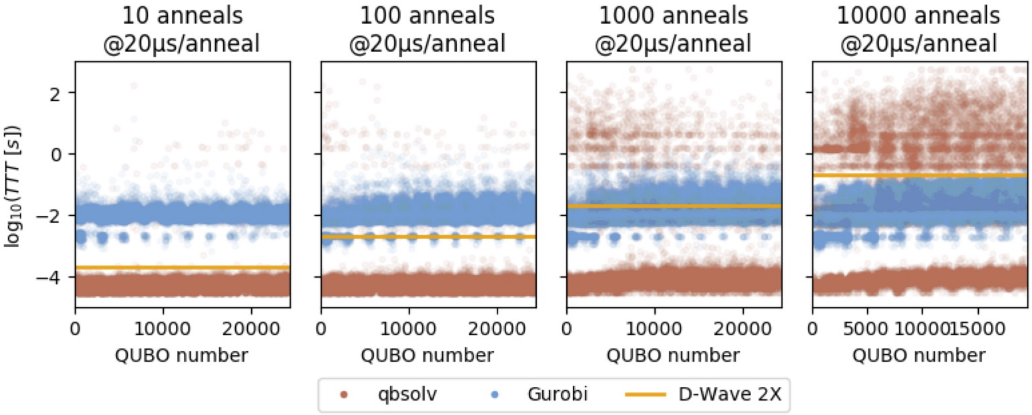
How to do it?

- Use “Alternating Least Squares”
    1. Randomly generate a binary C
    2. Solve $B = argmin_X ||A - XC||_F$ classically
    3. Solve $C = argmin_X ||A - BX||_F$ on the D-Wave
    4. Go to 2
- Step 3 is the interesting/D-Wave part
- In our analysis, A is 361×2491, B is 361×35 and C is 35×2491.
- C has $O(10^5)$ binary variables – far too many for the D-Wave, but...

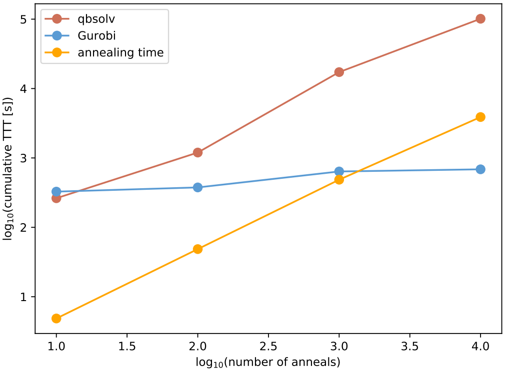
Step 3 in more detail

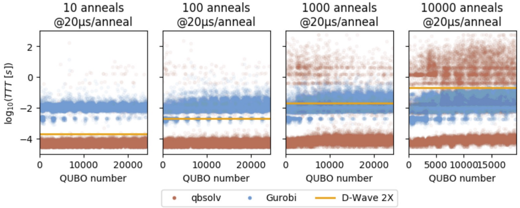
- $C = argmin_X ||A - BX||_F$ where C and X are 35×2491
- Step 3 is formulated above as a problem in 35×2491 binary variables, but it decomposes ("partitions") into 2491 problems with 35 binary variables each
- $C_i = argmin_x ||A_i - Bx||_2$ where C_i is the i^{th} column of C and x consists of 35 binary variables
- 35 binary variables fit on the D-Wave easily (can go to 49 with the VFYC)
- Imagine a Beowulf cluster of these...

What about performance?



What about performance?





- The D-Wave wins the cumulative time-to-targets modest number of anneals are used (up to 1000), but loses to Gurobi when 10,000 anneals are used
- qbsolv wins most problems, but loses very badly when it loses
- Gurobi takes too long to get rolling on the short time scales, but wins over longer times

Pros/cons: D-Wave NMF versus classical NMF

Forget the D-Wave and just view this as a method

Pros

- The D-Wave NMF's C matrix is $\sim 85\%$ sparse, but classical NMF's C matrix is only $\sim 13\%$ sparse
- The components of the D-Wave NMF's C matrix require fewer bits than classical NMF's C matrix (1 bit vs. 64 bits)
- Viewed as lossy compression, the D-Wave NMF compresses more densely

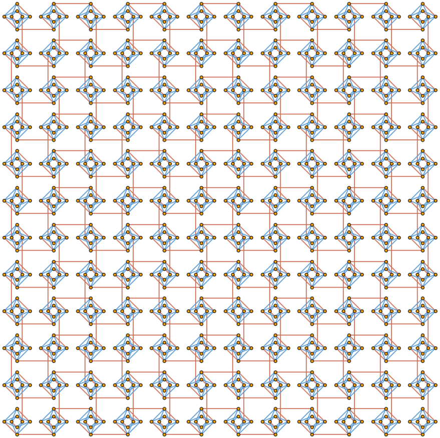
Cons

- Classical NMF's reconstructions have slightly less than half as much error as D-Wave NMF's reconstructions
- Viewed as lossy compression, the D-Wave NMF loses more information
- The B matrices are about 40% sparse for classical NMF, but dense for D-Wave NMF

Conclusions

- Utilized the D-Wave to solve a practical, unsupervised, machine-learning problem
- The D-Wave outperforms two state-of-the-art classical codes in a cumulative time-to-target benchmark when a low-to-moderate number of samples are used
  - Limitations in getting problems into/out of the D-Wave make these benefits hard to leverage, but the situation should improve with future D-Wave hardware
  - Custom heuristics would likely beat the D-Wave
- Large datasets can be analyzed on the D-Wave with this algorithm
  - We factored a 361×2491 matrix for consistency with Lee & Seung (Nature, 1999), but going larger is not a problem
- The D-Wave only limits the rank of the factorization
  - Not a major limitation, because we *want* the rank to be small

Preview: PDE-constrained optimization on the D-Wave



- 2D elliptic PDE that can be physically interpreted as representing heat transfer, mass diffusion, flow in porous media, *etc.*
- Use a custom embedding that leverages the virtual full yield chimera solver
- Gurobi can't keep up: even after 24 hours on 88 cores, Gurobi can't find a solution that matches the D-Wave's solution
- EES-16 Brownbag: May 11 @ noon in the EES-16 conference room (Otowi)