JUNIQ/EPIQ Summer School on Quantum Computing

Topic 5 - QSVM

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QSVM

Construction

- An SVM is a supervised machine-learning method for binary classification
- Given a training set

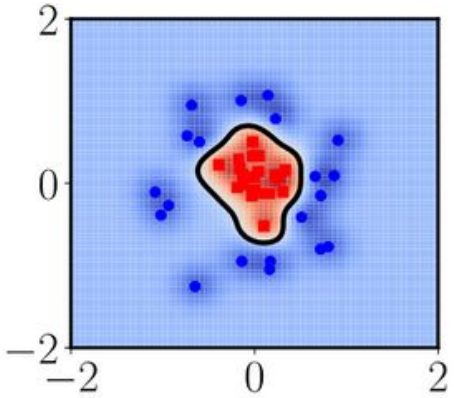
Feature vector — Label

$$D = \{(\mathbf{d}_n, t_n) : n = 0, \ldots, N-1\}$$

an SVM is trained by solving the Quadratic Programming problem

$$\text{minimize} \qquad E(\{\alpha_n\}) = \frac{1}{2}\sum_{nm} \alpha_n \alpha_m t_n t_m k(\mathbf{d}_n, \mathbf{d}_m) - \sum_n \alpha_n$$

$$\text{subject to} \qquad 0 \le \alpha_n \le C \quad \text{and} \quad \sum_n \alpha_n t_n = 0$$



Continuous problem variables

Kernel function (nonlinear SVM)

- QUBO problems are also quadratic, but for binary variables

Number of qubits per problem variable

→ Use encoding: $\alpha_n = \sum_{k=0}^{K-1} B^{k-P} x_{[n,k]}$

Base & Exponent

$\rightarrow E(\{\alpha_n\})$

QUBO formulation

$$\min_{x_i=0,1} \left(\sum_{i,j} x_i Q_{ij} x_j \right)$$

QSVM

Construction

The upper bound is taken on when all bits are 1, corresponding to

$$C = \sum_{k=0}^{K-1} B^{k-P}.$$

We then insert the encoding into the energy

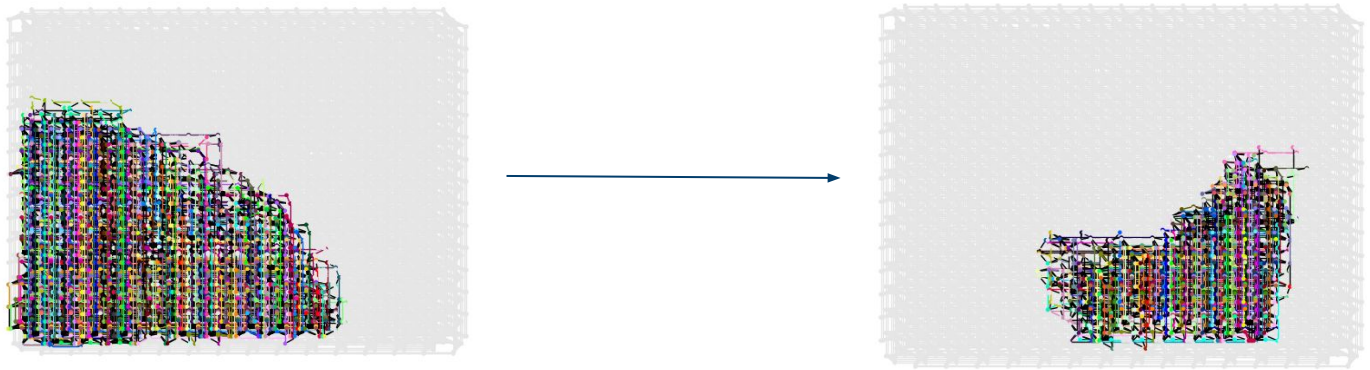
$$E(\{\alpha_n\}) + \frac{\xi}{2}\left(\sum_n \alpha_n t_n\right)^2,$$

where ξ is a Lagrange multiplier to incorporate the equality constraint of the SVM problem into our QUBO, and collect all linear and quadratic terms in the $\{x_{n,k}\}$. This yields the SVM problem in QUBO formulation

$$\min\left(\sum_{n,m=0}^{N-1}\sum_{k,j=0}^{K-1} x_{n,k}\, Q_{n,k;m,j}\, x_{m,j}\right),$$

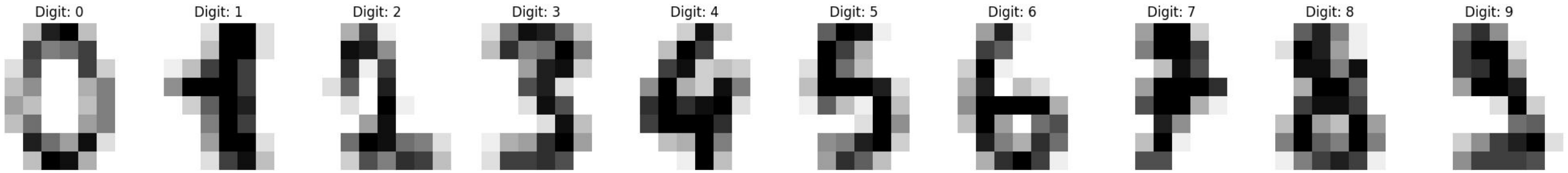
with the resulting $NK \times NK$-dimensional QUBO matrix (*Note*: Doing this calculation is a nice optional exercise ;-)):

$$\texttt{Q[f'x\{n\},\{k\}', f'x\{m\},\{j\}']} = \frac{1}{2}B^{k+j-2P} t_n t_m \left(\mathrm{rbf}(\vec{d}_n, \vec{d}_m) + \xi\right) - \delta_{nm}\delta_{kj} B^{k-P}.$$



MNIST

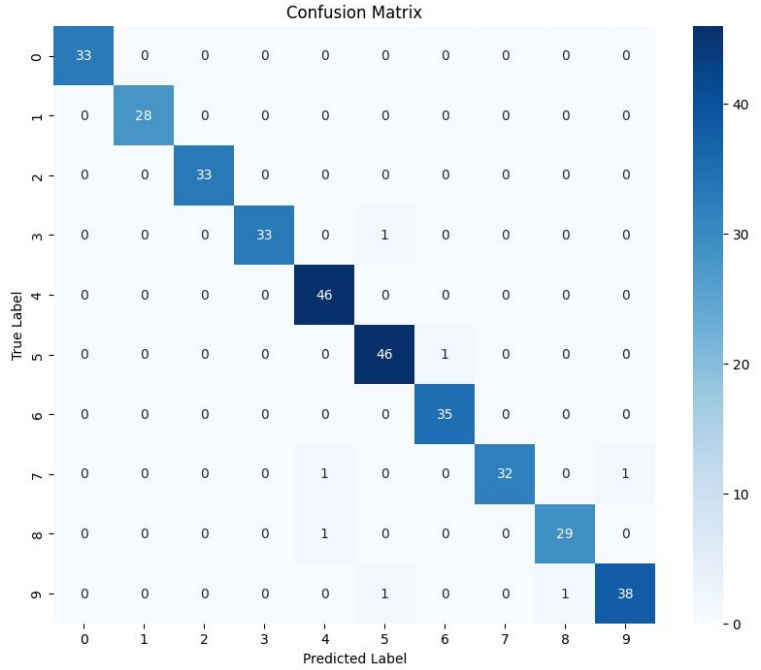
- Dataset of handwritten numbers
  - Numbers from 0 to 9
- 8x8 resolution
- 1.797 pictures

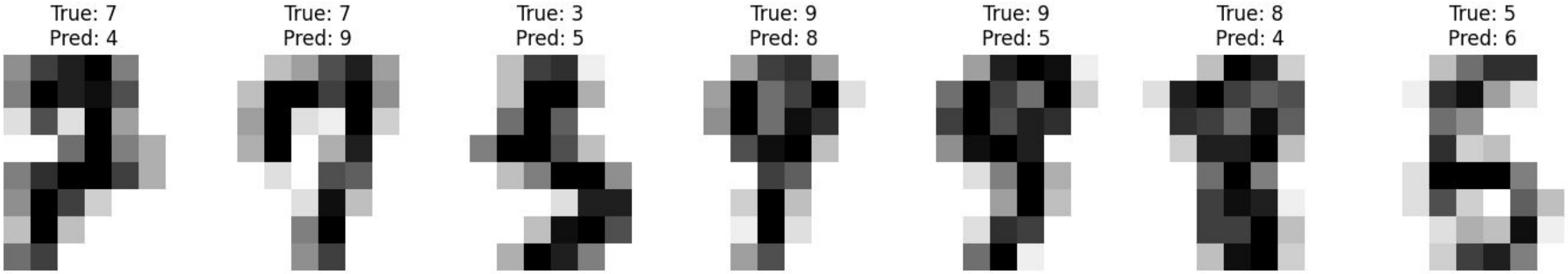


Classic SVM

https://colab.research.google.com/drive/1fUeycuGlflf1fS7xjzUKKNy4H-yh-UQK?usp=sharing

- With Radial Basis Function (RBF)
- Multiclass → O v O
- Accuracy: 0.9806 (98.06%)





QSVM

Binary Classification

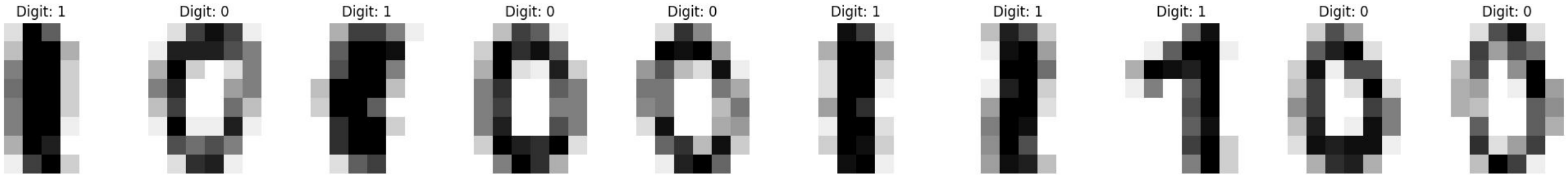
- Binary labels: 0 and 1 mapped to → +1 and -1
- Reduces Qubo size, and `response = sampler.sample_qubo(Q, num_reads=500)`

Hyperparameters

- B=[2]
- K=[3]
- xi=[1]
- gamma=[1]

- Performs worse that our classical SVM

```
[gen_svm_qubos] mnistcalibtrain0 unique labels: [-1.  1.]
Creating the QUBO of size (486, 486)
Extracting nodes and couplers
Saving 486 nodes and 117855 couplers for outputs/calibration3/mnist/runmnistcalibtrain0_B=2_K=3_xi=1_
a=1/
running outputs/calibration3/mnist/runmnistcalibtrain0_B=2_K=3_xi=1_gamma=1/result_couplers=117855/ w
486 nodes and 117855 couplers
 -- no embedding found, removing outputs/calibration3/mnist/runmnistcalibtrain0_B=2_K=3_xi=1_gamma=1/
lt_couplers=117855/ and trying fewer couplers
running outputs/calibration3/mnist/runmnistcalibtrain0_B=2_K=3_xi=1_gamma=1/result_couplers=2500/ wit
6 nodes and 2500 couplers
idx     sum_antn        trainacc        trainauroc      trainauprc      testacc         testauroc
estauprc
0       -9.0000         0.8086          1.0000          1.0000          0.5062          0.9994
0.9994
0       -9.0000         0.8086          1.0000          1.0000          0.5062          0.9994
0.9994
1       -5.0000         0.7901          1.0000          1.0000          0.5000          0.9992
0.9993
1       -5.0000         0.7901          1.0000          1.0000          0.5000          0.9992
0.9993
2       -6.0000         0.7778          0.9998          0.9998          0.5062          0.9992
0.9993
2       -6.0000         0.7778          0.9998          0.9998          0.5062          0.9992
0.9993
3       -19.0000        0.8519          1.0000          1.0000          0.5062          0.9991
0.9991
3       -19.0000        0.8519          1.0000          1.0000          0.5062          0.9991
0.9991
4       -20.0000        0.8210          1.0000          1.0000          0.5062          0.9989
0.9990
4       -20.0000        0.8210          1.0000          1.0000          0.5062          0.9989
0.9990
5         9.0000        0.8580          1.0000          1.0000          0.4938          0.9991
0.9991
5         9.0000        0.8580          1.0000          1.0000          0.4938          0.9991
0.9991
6       -15.0000        0.8457          1.0000          1.0000          0.5062          0.9994
0.9994
6       -15.0000        0.8457          1.0000          1.0000          0.5062          0.9994
```



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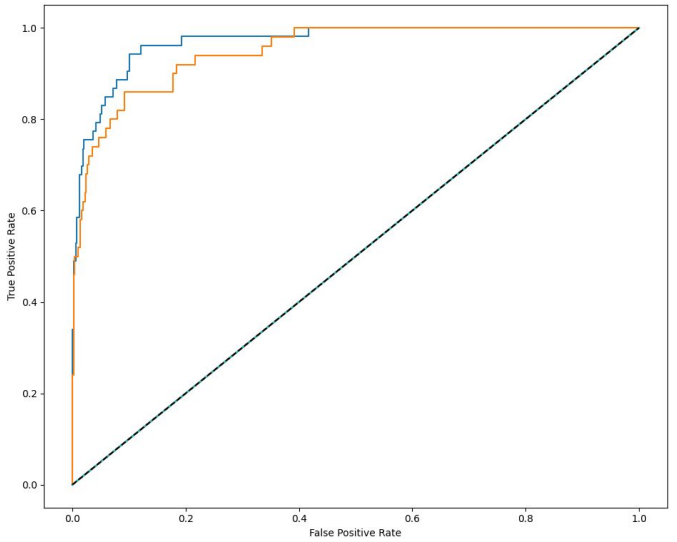
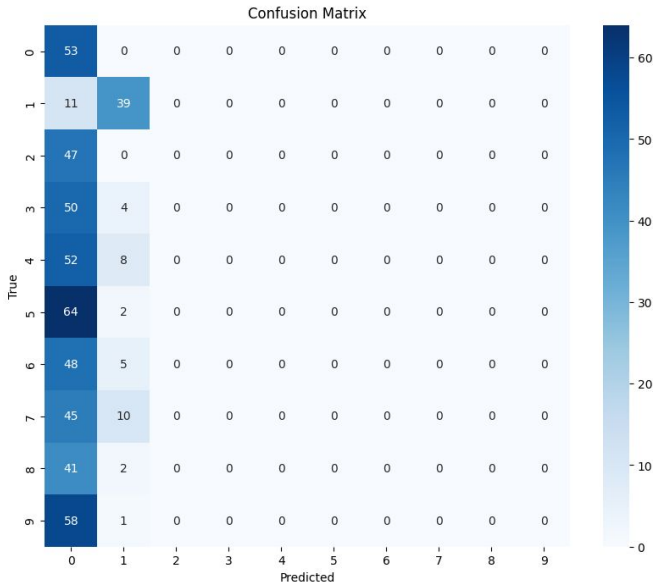
QSVM

Multi Class Classification

- Using the same Dataset with Multi Class Classification on DWave with nreads = 10000
  - SolverFailureError: The problem cannot be submitted because its estimated QPU access time of 2773392 microseconds exceeds the maximum of 1000000 microseconds for Advantage_system4.1.

- OneVsAll approach on digits 0,1,2.
  - nreads = 2000





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