QuCOOP: A Versatile Framework for Solving Composite and Binary-Parametrised Problems on Quantum Annealers

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Motivation

Solve

$$\underset{x\in\{0,1\}^k,\, g(x)\in\mathcal{S}}{\arg\min}\; f(g(x)), \quad (1)$$

$$f(g(x)) = \langle g(x), \mathbf{Q}g(x) + \mathbf{c}\rangle\,, \quad (2)$$

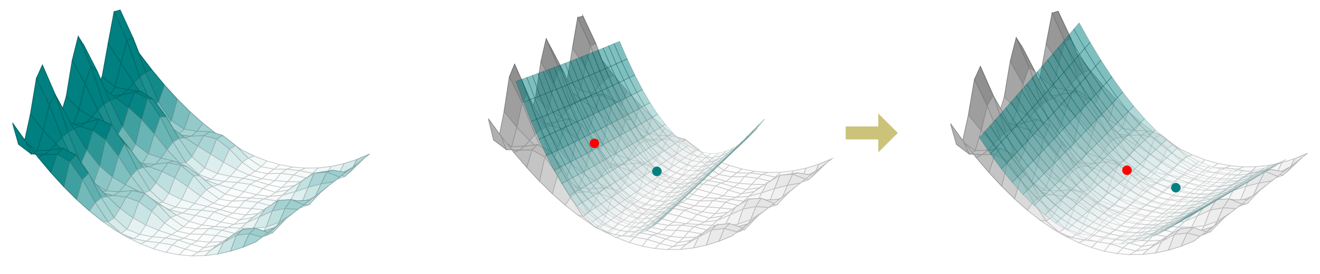
for some feasible set $\mathcal{S}\subset\mathbb{R}^n$.

From Discrete to Quantum

Challenge: Problem (1) is a discrete problem.

Idea: Could be tackled on quantum annealer.

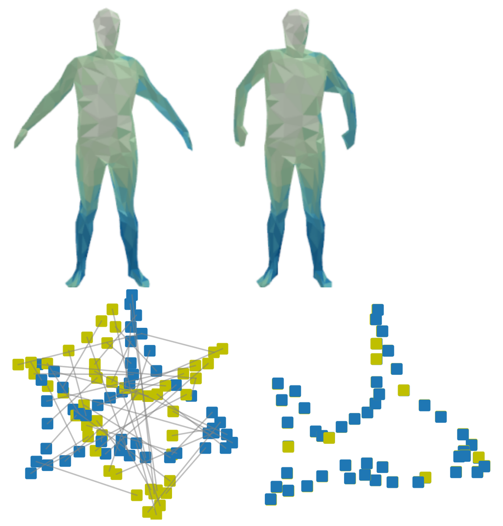
Challenge: Problem (1) is not a QUBO.



(a) **Minimise** $f(g(x))$
f quadratic in $g(x)$: ✔,
x binary: ✔, g linear in x: ✘
AQC: ϟ **Not a QUBO !!!**

Minimise $f(g^t(x) := g(x^t) + \langle \nabla g(x^t), x - x^t\rangle)$
f quadratic in $g^t(x)$: ✔,
x binary: ✔, g^t linear in x: ✔
AQC: ✔ **Iteratively solve QUBOs !!!**

Example Applications



Shape matching:

$$\underset{\mathbf{P}\in\Pi_n}{\arg\min}\; \|\mathbf{AP} - \mathbf{PB}\|_F^2, \quad \text{(SM)}$$

where $\mathbf{P}$ can be expressed as a function of binary variables.

Point set registration:

$$\underset{\mathbf{R}\in SO(d),\, \mathbf{P}\in\Pi_n}{\arg\min}\; \|\mathbf{XP} - \mathbf{RY}\|_F^2, \quad \text{(PSR)}$$

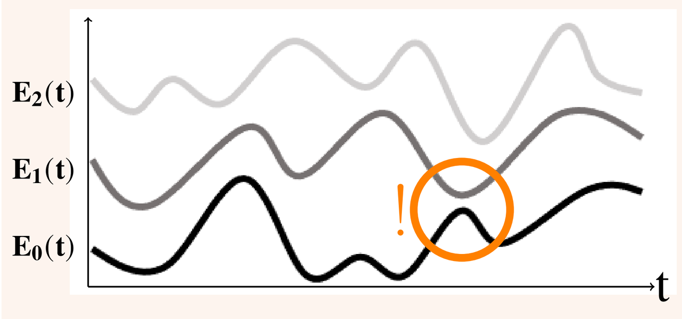
where $\mathbf{R}$ and $\mathbf{P}$ can be expressed as functions of binary variables.

Adiabatic Quantum Computing (AQC)

Quantum annealers can solve Quadratic Unconstrained Binary Optimisation (QUBO) problems:

$$\underset{x\in\{0,1\}^n}{\arg\min}\; \langle x, \mathbf{Q}x + \mathbf{c}\rangle\,, \quad (3)$$

where $\langle\cdot,\cdot\rangle$ is the standard inner product in $\mathbb{R}^n$, $\mathbf{Q}$ a symmetric matrix, and $\mathbf{c}$ a vector [1].



They rely on the Schrödinger equation

$$i\hbar\frac{\partial\,|\psi(t)\rangle}{\partial t} = H(t)\,|\psi(t)\rangle\,, \quad t\in[0,T], \quad (4)$$

$$H(t) = -(1-\frac{t}{T})\underbrace{\left(\sum_{i=1}^{n}\sigma_i^x\right)}_{=:H_i} - \frac{t}{T}\underbrace{\left(\sum_{i,j=1}^{n} Q_{ij}\sigma_i^z\otimes\sigma_j^z + \sum_{i=1}^{n} c_i\sigma_i^z\right)}_{=:H_p}.$$

Adiabatic theorem: If t varies slowly enough, the evolution of the system will instantaneously keep the state $|\psi(t)\rangle$ into the ground state $|E_0(t)\rangle$ of $H(t)$, which is at $t = T$ the solution of the QUBO.

QuCOOP: COmposite OPtimisation on QUantum Annealers

Algorithm

Initialize x^0 and repeat for $t = 0, 1, 2, \ldots$

$$g^t(x) := g(x^t) + \left\langle \nabla g(x^t), x - x^t\right\rangle \quad (5)$$

$$x^{t+1} \leftarrow \underset{x\in\mathbb{B}^k}{\arg\min}\; \left\{f^t(x) := f(g^t(x))\right\} \quad (6)$$

$$\text{s.t.}\quad g^t(x)\in\mathcal{S} \quad (7)$$

Equivalent QUBO

In each iteration t, solve

$$\underset{x\in\{0,1\}^k}{\arg\min}\; \left\langle x, \mathbf{Q}^t x + \mathbf{c}^t\right\rangle + \text{PenaltyTerm}(g(x^t)),$$

$$\mathbf{Q}^t := \nabla g(x^t)\mathbf{Q}\nabla g(x^t)^\top,$$

$$\mathbf{c}^t := \nabla g(x^t)\Big(\mathbf{c} + 2\mathbf{Q}\Big(g(x^t) - \nabla g(x^t)^\top x^t\Big)\Big).$$

Application to Shape Matching and Point set Registration

Binary parametrisation of permutations: Any permutation matrix $\mathbf{P}\in\Pi_n$ can be parametrised with a length-k, $k = n(n-1)/2$, binary vector $x := (x_1, \ldots, x_k)$ via the function

$$\mathbf{P}(x) := \prod_{i=1}^{k}\mathbf{P}_i(x_i), \quad \mathbf{P}_i(x_i) := \mathbf{T}_i^{x_i}, \quad (8)$$

where $\mathbf{T}_i^{x_i}$ is the ith transposition from $((a,b),\ a,b = 1,\ldots,n,\ a<b)$ if $x_i = 1$ and $\mathbf{I}_{n\times n}$ otherwise.

Illustration: $(c, d, b, a) \to (\mathbf{a}, d, b, c) \to (\mathbf{a}, \mathbf{b}, d, c) \to (\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d})$

Fix position 1 / Transpose (1, 4) — Fix position 2 / Transpose (2, 3) — Fix position 3 / Transpose (3, 4) — Done

$$\mathbf{P} = (3,4)^1\cdot(2,4)^0\cdot(2,3)^1\cdot(1,4)^1\cdot(1,3)^0\cdot(1,2)^0$$

Binary parametrisation of rotations: Any rotation matrix in $SO(d)$ can be parametrised as

$$\mathbf{R}(y) = \exp(\mathbf{M}(y)), \quad \mathbf{M}(y) = \begin{pmatrix}0 & -y\\ y & 0\end{pmatrix}\ \textbf{in 2D}, \quad \mathbf{M}(y) = \begin{pmatrix}0 & -y_3 & y_2\\ y_3 & 0 & -y_1\\ -y_2 & y_1 & 0\end{pmatrix}\ \textbf{in 3D}. \quad (9)$$

Trick: Write $y_i = a\cdot\sum_i 2^i q_i$, $\quad q_i\in\{0,1\}$ and refine discretisation interval: $[+++] \to [\,\|\|\|++]$ ($y_i^{t+1}\, y_i^t \to y_i^t$)

QuCOOP as Applied to SM and PSR

Set $\mathbf{p}(x^t) + \langle\nabla\mathbf{p}(x^t), x - x^t\rangle$ and $\mathbf{r}^t(y) = \mathbf{r}(y^t) + \langle\nabla\mathbf{r}(y^t), y - y^t\rangle$. In each iteration t:

$$\text{(SM)} \Leftrightarrow \underset{x\in\{0,1\}^k}{\arg\min}\; \langle g^t(x), \mathbf{Q}g^t(x)\rangle + \square,$$

$$\mathbf{Q} := \alpha\mathbf{I}_{n\times n} - \mathbf{A}\otimes\mathbf{B},$$

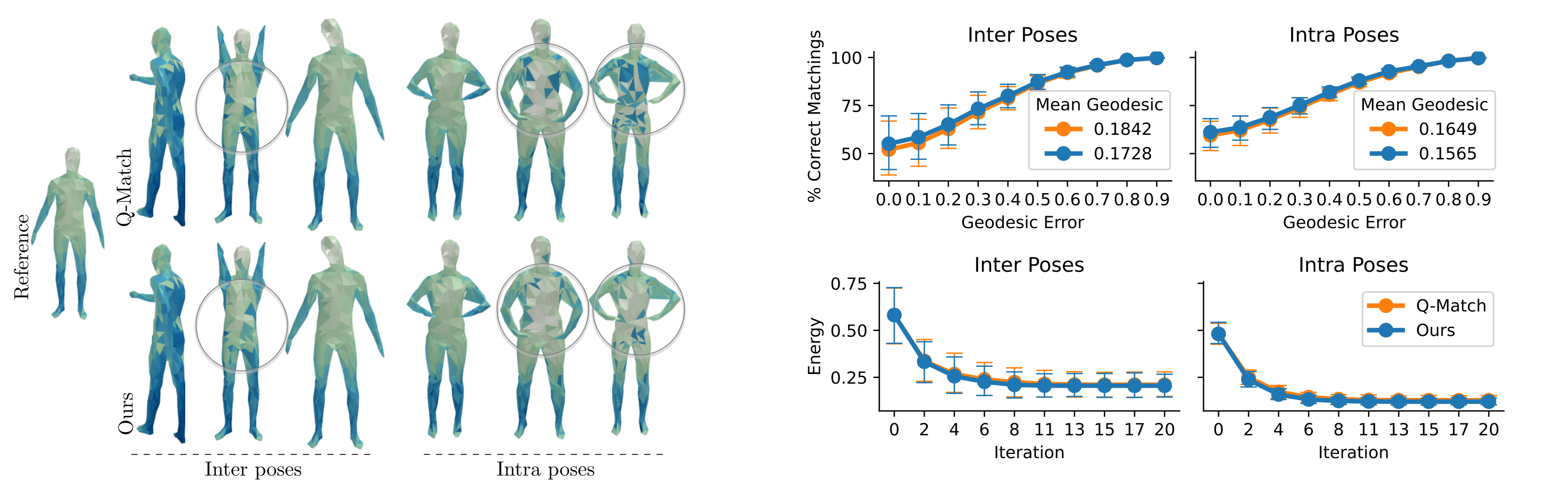
$$\text{(PSR)} \Leftrightarrow \underset{(x,y)\in\{0,1\}^k}{\arg\min}\; \langle g^t(x,y), \mathbf{Q}g^t(x,y)\rangle + \square,$$

$$\mathbf{Q} := \begin{pmatrix}\alpha\mathbf{I}_{n\times n} & -\frac{1}{2}\mathbf{X}\otimes\mathbf{Y}\\ -\frac{1}{2}(\mathbf{X}\otimes\mathbf{Y})^\top & \beta\mathbf{I}_{d\times d}\end{pmatrix},$$

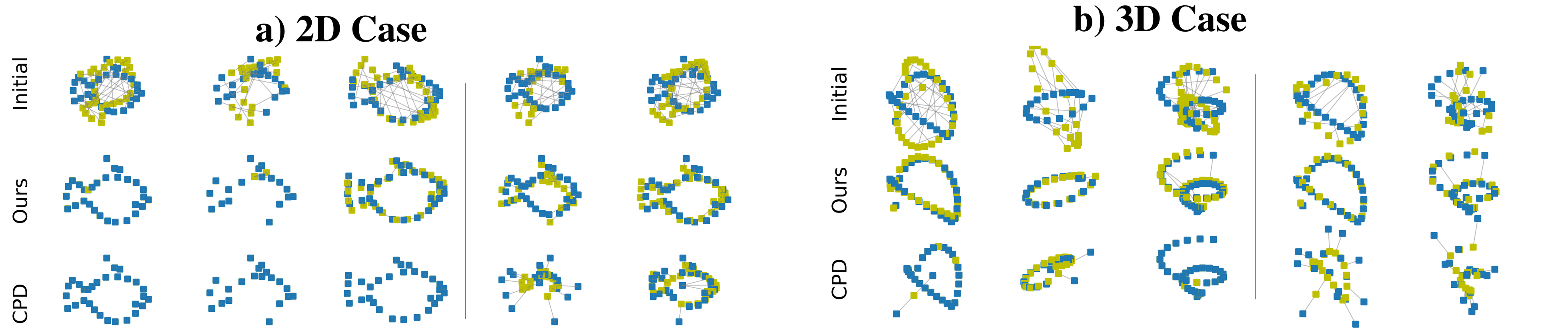
With $g^t(x) =: \mathbf{p}^t(x)$ in (SM), $g^t(x,y) := (\mathbf{p}^t(x), \mathbf{r}^t(y))$ in (PSR) and $\square := \alpha\cdot\|(g^t(\cdot))\|^2,\ \alpha\in\mathbb{R}_+$.

Results

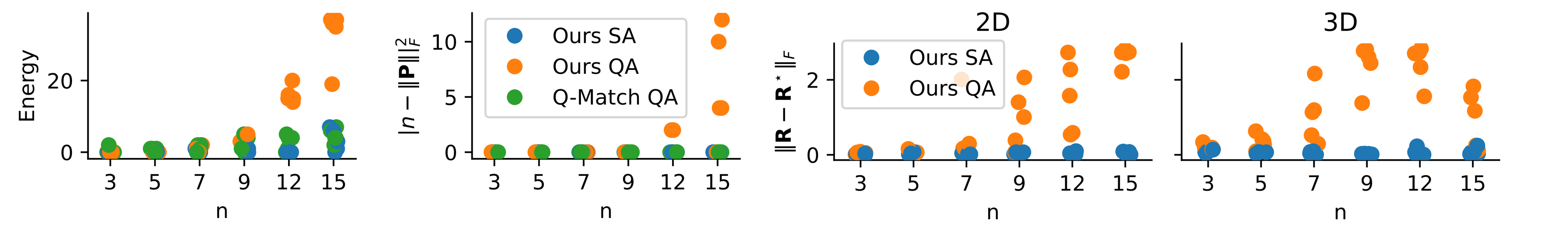
I. Shape Matching using Simulated Annealing (vs. Q-Match [3])



II. Point Set Registration using Simulated Annealing (vs. CPD [4])



III. Results on D-Wave Quantum Annealers [2]



Summary:

- QuCOOP extends the scope of AQC to some form of non-quadratic problems, see Problem (1).
- QuCOOP is able to handle problems involving permutations/assignments.
- QuCOOP is versatility and compatibility with continuous problems such as in (PSR) .

References

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[2] D-Wave Systems. QPU Solver Datasheet. https://docs.dwavesys.com/docs/latest/doc_qpu.html, 2024.

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[4] Myronenko, Andriy and Song, Xubo. Point Set Registration: Coherent Point Drift. *PAMI*, 90(1), 2010.