Quantum-Inspired Optimization based on Digital Annealer

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Agenda

- Introduction: Quantum Inspired Computing
- Use Cases
- Qubo-Building / Tutorial
- Q&A
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- Introduction: Quantum Inspired Computing
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Finding the way through Hard Problems

Guided by a flashlight

Guided by a lantern
Conventional Systems (CPUs / GPUs) | The Flashlight

Calculation of one (CPU) or some (GPU) solution path(s) at a time (one direction)
Quantum Computers | The Lantern

Light up the entire landscape to decide which direction to go (all possibilities at the same time)
But: Quantum Computing will not be a General Purpose approach. It will be used where it provides RoI and/or enables a competitive advantage.

- **Stability**
  - Isolation from magnetic field
  - Error correction

- **Complex Infrastructure & Cost**
  - Isolating from any external interference
  - Running at milli-Kelvin degrees

- **Accuracy**
  - Qubits tend to lose superposition state

- **Readiness**
  - Network latency
  - Solve real world problems (?)
When the solution space grows exponentially,...

PVC sealing robot optimization

<table>
<thead>
<tr>
<th>n (number of seams)</th>
<th>2</th>
<th>7</th>
<th>10</th>
<th>23</th>
<th>65</th>
</tr>
</thead>
<tbody>
<tr>
<td>$2^{n-1}(n-1)!$ combinations</td>
<td>2</td>
<td>46,080</td>
<td>$1.86 \times 10^8$</td>
<td>$4.71 \times 10^{27}$</td>
<td>$2.34 \times 10^{108}$</td>
</tr>
<tr>
<td>$2(n-1)^2$ bits on Q-Systems</td>
<td>2</td>
<td>72</td>
<td>162</td>
<td>968</td>
<td>8192</td>
</tr>
</tbody>
</table>

Potential sweetspots for Digital Annealer

- **Real time requirements:** Same solution, faster
- **Quality requirements:** Same time, better solution
- **Disruptive requirement:** Find (good) solution at all

Optimization Technology

- Quantum Computer
- **Real time**
- CPU/GPU

- Small problem space
- Large space
- Too slow, limited

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FUJITSU Quantum-Inspired Optimization Services

An available future-proof Bridge to Quantum Computing

- Inspired by Quantum Parallelism (Superposition)
  - Digital Annealer evaluates all subsequent candidate states, arising from all 8192 possible bit flips, in parallel

- Inspired by Quantum Entanglement
  - The full-connectivity of Digital Annealer facilitates near instant interaction across the whole system state

- Inspired by Quantum Tunnelling
  - Unique architecture simultaneously evaluates multiple energy potentials, akin to Quantum Tunneling in quantum annealing, accelerating convergence
Quantum Inspired: FUJITSU Digital Annealer

**Differentiators**

- Full connectivity through the 8192 bit scale, **16-64-bit precision**
- Provides the ability to represent a **large scale problem effectively**

**Easy Problem Mapping**

- **8192-bit scale**
- **Bit 8192**
- **Bit i (Full connectivity)**

**Parallel Speed up**

- **Parallel processing** making it much faster than standard computing
- Stochastic parallelism providing significant **speed up**

**Annealing Process**

- **DA increases escape probability** from the local minimum energy state with the hardware offsetting
- **Faster** than traditional simulated annealing
What is Annealing?

- Not annealing:
  - Run by trial and error through all combinations
  - Huge number of steps (“n!”)

- Annealing:
  - Shake heavily & let fall
  - Shake less & let fall ...
  - Stable solution after “few” rounds

- Annealing of sword:
  - Shake = heat, fall = hammer
  - stable = durable
Comparison of Annealing Technologies

- **Simulated Annealing**
  - 99% global optimum
  - Slow
  - Large search space
  - No Quantum Ecosystem

- **Digital Annealer**
  - 99% global optimum
  - Real Time
  - Large search space
  - Quantum Ecosystem

- **Quantum Annealer**
  - 100% global optimum
  - Real Time
  - Small(est) search space
  - Quantum Ecosystem
Discover Optimum by Annealing

For a set of possible combinations …

… define a search space and energy function …

\[
E(x) = \sum_{p=0}^{N-1} \left( 1 - \sum_{l=0}^{N-1} x_{p,l} \right)^2 + \ldots
\]

Digital Annealer finds minimum of energy function

… whose minimum is the best fitting solution.
Quantum Computing & Annealing

- Simulated Annealing
- Digital Annealer
- Quantum Annealer
- Quantum Gate Computer

Search for minimum energy

$E(x)$ real function

$E(X) = \sum_{i=1}^{N} b_i x_i + \sum_{i=1}^{N} \sum_{j=1}^{i-1} w_{ij} x_i x_j$ binary polynomial

Classical hardware

Special hardware

Quantum Annealer

Quantum Gate HW

All

Fujitsu

D-Wave

e.g. Google, IBM

1) Source: www.dwavesys.com
2) Source: www.inceptivemind.com
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Noise Suppression

Use Case with a German car manufacturer

- Optimization of the shape of side mirrors or other car parts for minimum noise emission
- Digital Annealer is able to calculate an optimal shape for complete noise suppression
- Digital Annealer can reduce the sound to 0 dB

<table>
<thead>
<tr>
<th>$d$ (Displacements) ^ n (Pos.)</th>
<th>$3^2$</th>
<th>$3^{25}$</th>
<th>$g^{122}$</th>
<th>$g^{1000}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(d)^n$ Combinations</td>
<td>8</td>
<td>$8.47 \times 10^{11}$</td>
<td>$1.5 \times 10^{110}$</td>
<td>$1.23 \times 10^{903}$</td>
</tr>
</tbody>
</table>

Quantum Technology

- Quantum Annealing
- Digital Annealer
De Novo Digital Drug Design

- Combination of quantum-inspired technology, machine learning and simulations in the development of new molecule candidates
- Finding new drug candidates by expanding the searchable chemical space from 0.5 - 10 million molecules (market standard) to billions
- Reduction of the total time needed to find de novo drugs from 24-48 months to about 8 months
### Job Shop Scheduling

- Production jobs are sequential operations on machines.
- Some jobs require multiple operations on a single machine and each job may require different sequencing of operations.
- Digital Annealer computes runtime in less than a second.

<table>
<thead>
<tr>
<th>$j \times m$ possibilities</th>
<th>$3 \times 3$</th>
<th>$5 \times 5$</th>
<th>$10 \times 10$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(j^3)^m$</td>
<td>216</td>
<td>$2.48 \times 10^{10}$</td>
<td>$3.95 \times 10^{65}$</td>
</tr>
</tbody>
</table>

Quantum Technology:  
- Quantum Annealing
- Digital Annealer
Challenges | Solved today with Digital Annealer

Financial
Enabled the bank to achieve a well diversified portfolio. Demonstrated 300 times faster results compared to their existing systems

Pharmaceuticals
Accelerated protein structure prediction for drug discovery and biotech research. The most stable structures were identified from $10^{100}$ candidates in minutes

Manufacturers
Executing job-shop rescheduling in 1 second.
Reduce travel distance for picking warehouse parts by up to 45%

Global automotive OEM
Large Automotive OEM successfully optimized mirror design of the car to eliminate noise emission for improved driving comfort

Automotive OEM
European Automotive OEM successfully optimized robot positioning for 64seam sealing of chassis, resulting in production of more cars with the same resources and time

Japan Post
Shrinking delivery fleet, time and cost. Improved loading efficiency by optimizing transportation scheduling of parcel delivery trucks
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Daily NP-Hard Problem

What combination of clothes...

...fits best!
Formalised decision model

Choice bit matrix

\[ X = (x_{p,c}) \]

If choice \( c \) for piece \( p \)
then
\[ x_{p,c} = 1 \]
else
\[ x_{p,c} = 0 \]
Formalised decision model

Choice bit matrix

\[ X = (x_{p,c}) \]
Formalised decision model

Choice bit matrix

\[ X = (x_{p,c}) \]

<table>
<thead>
<tr>
<th></th>
<th>choice c</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1</td>
</tr>
<tr>
<td>( x_{p,c} )</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td>0</td>
</tr>
</tbody>
</table>

1 = \( \checkmark \)
Mathematical model - best fit

Evaluation of the selection $X$

$$F(X) = \sum p = 1, 2, \ldots$$

Not Selected!

Not Selected!
Mathematical model - best fit and restrictions

Evaluation of the selection $X$

$$F(X) = \begin{cases} 1 & \text{if } \sum_{i=1}^{n} x_i = p, c_1 x_i = c_2 \\
0 & \text{otherwise} \end{cases}$$

Mathematical energy formula (QUBO) completed!

The rest is done by ... Digital/Quantum Annealing
Digital Annealer finds the minimum = solution

Minimize: \( E(X) = P(X) - F(X) \)

\[
E(X) = \sum_{p=1}^{3} \sum_{c_1, c_2 \in \{1, 2, 3\}, c_1 \neq c_2} \alpha \cdot x_{p,c_1} x_{p,c_2} - \sum_{p=1}^{3} \sum_{c_1=1}^{3} \sum_{c_2=1}^{3} f_p(c_1, c_2) x_{p,c_1} x_{p+1,c_2}
\]

Solution: \( X_{\text{min}} \)

\[
X_{\text{min}} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \end{bmatrix}
\]
Inside the Digital Annealer

Mathematical model:

\[ E(X) = \sum_{p=1}^{3} \sum_{c_1, c_2 \in \{1, 2, 3\}, c_1 \neq c_2} a \cdot \alpha_{c_1, c_2} \cdot \left( f_p(c_1, c_2) - \sum_{p=1}^{2} \sum_{c_1=1}^{3} \sum_{c_2=1}^{3} f_p(c_1, c_2) \cdot \right) \]
Inside the Digital Annealer

Mathematical model:

\[ E(X) = \sum_{p=1}^{3} \sum_{c_1, c_2 \in \{1,2,3\}, c_1 \neq c_2} \alpha x_{p,c_1}x_{p,c_2} - \sum_{p=1}^{2} \sum_{c_1=1}^{3} \sum_{c_2=1}^{3} f_p(c_1,c_2)x_{p,c_1}x_{p+1,c_2} \]

Energy Map:

What is the current combination?

DA starts with random 0-1 combinations
Inside the Digital Annealer

Mathematical model:

\[ E(X) = \sum_{p=1}^{3} \sum_{c_1, c_2 \in \{1,2,3\}}^{\alpha} x_{p,c_1} x_{p,c_2} - \sum_{p=1}^{2} \sum_{c_1=1}^{3} \sum_{c_2=1}^{3} f_p (c_1, c_2) x_{p,c_1} x_{p+1,c_2} \]

Energy Map:

- Improvements are always accepted!
- The worse combinations are deleted

Parallel!
Inside the Digital Annealer

Mathematical model:

\[
E(X) = \sum_{p=1}^{3} \sum_{c_1, c_2 \in \{1, 2, 3\}, c_1 \neq c_2} \alpha \ x_{p,c_1} x_{p,c_2} - \sum_{p=1}^{2} \sum_{c_1=1}^{3} \sum_{c_2=1}^{3} f_p(c_1, c_2) x_{p,c_1} x_{p+1,c_2}
\]

What does "Annealing" mean?

Annealing ...
Current combination

\[
E = \begin{pmatrix}
1 & 2 & 3 \\
4 & 5 & 6
\end{pmatrix}
\]

New combination

\[
E = \begin{pmatrix}
7 & 8 & 9 \\
10 & 11 & 12
\end{pmatrix}
\]

Accept?

~coin toss
frequently

~ Dice
seldom

~ Lotto
Almost never

Energy Map:

Duration = Annealing Temperature drop

\[
E(X)
\]

Annealing

\[\times\]
Inside the Digital Annealer

Mathematical model: 
\[
E(X) = \sum_{p=1}^{3} \sum_{c_1, c_2 \in \{1,2,3\}, c_1 \neq c_2} \alpha x_{p,c_1} x_{p,c_2} - \sum_{p=1}^{2} \sum_{c_1=1}^{3} \sum_{c_2=1}^{3} f_p(c_1, c_2) x_{p,c_1} x_{p+1,c_2}
\]

What does "Annealing" mean?

Why Annealing ...

Mathematical model \( E(X) \)

- Local minimum in the energy model \( E(X) \)
  - Temperatures allow to come out!
- Low local minimum at the end of the term
  - Temperatures too low to get out
- No improvement: Waiting time depending on temporary increase from (Lotto) to (Coin)

Duration = Annealing
Temperature drop

Energy Map:

- Low energy state
- High energy state
- Transition points

https://images.unsplash.com/photo-1550751627-4bd3743f58b?ixlib=rb-1.2.1&ixid=eyJhcHBfaWQiOjEyMDd9&auto=format&fit=crop&w=1350&q=80

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Live Demonstration

PC / Jupyter Notebook

Digital Annealer Cloud
Digital Annealer Tutorials

Try out our Digital Annealer tutorials for yourself!

Apply for your access via

www.fujitsu.com/de/themes/digitalannealer/get-started/

These tutorials are waiting for you

- Seating Optimization - compliance with the currently required minimum distance in the office
- Workforce Scheduling - Optimal design of shift planning
- Dial-a-Ride - Optimal distribution of a taxi fleet/ transport fleet to incoming orders
- Timetables - optimal timetable for students, teachers and lesson content

Deep Dive Tutorials

- How does the FUJITSU Optimizer work (UI function, widgets, logging)?
- What are polynomials, variables and cost functions and how do you calculate with them?
- How does annealing, parallel tempering and sampling work?
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