

# QuantumGEP: Gene Expression Programming for Quantum Computing

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A person with dark hair, wearing a blue and black plaid shirt and purple nitrile gloves, is working on a complex piece of scientific equipment. The equipment is a quantum circuit device, possibly a superconducting qubit system, with various wires and components. The person is looking intently at the device, which is illuminated by a bright light source. The background is dark, suggesting a laboratory setting.

## Motivation: Find Quantum Circuits

✂ Which quantum circuits do we want?

Those that when applied to an initial state yield the ground state of a Hamiltonian

A person with dark hair, wearing a blue and black plaid shirt and purple nitrile gloves, is focused on adjusting a red component of a quantum computing setup. The setup includes a large, dark cylindrical cryostat and various wires and cables. The background is a plain, light-colored wall.

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✂ Why? In order to use **quantum computing** in Condensed Matter, Graph Theory, and Quantum Chemistry

A person with dark hair, wearing a plaid shirt and purple gloves, is working with a quantum computing setup. They are holding a red component connected to various wires and a large metal cryostat. The background is a laboratory setting with a yellow wall.

## Motivation: Find Quantum Circuits

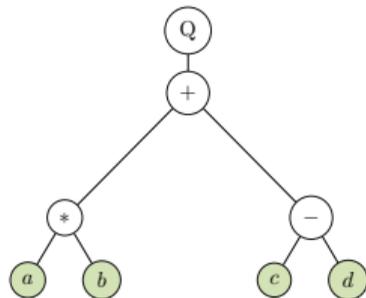
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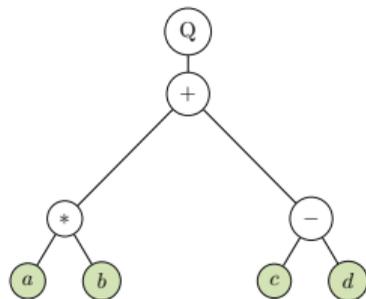
✂ QuantumGEP can produce thousands of circuits, with hundreds correct; it produces non-parametric circuits

## Gene Expression Programming Overview

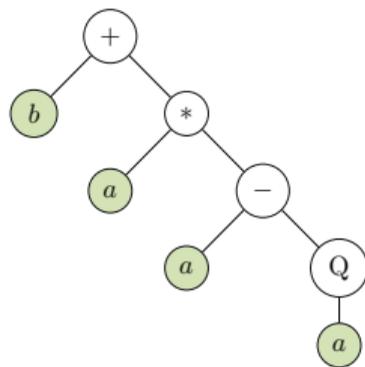


Abstract Syntax Tree (AST) for  $\sqrt{a * b + (c - d)}$ , with string representation  $Q+^*-abcd$ , operator (or primitives) in  $\{Q, +, -, *\}$ , and leaves (shaded in the figure) in  $\{a, b, c, d\}$ .  
Order is **breadth first**. No parenthesis!

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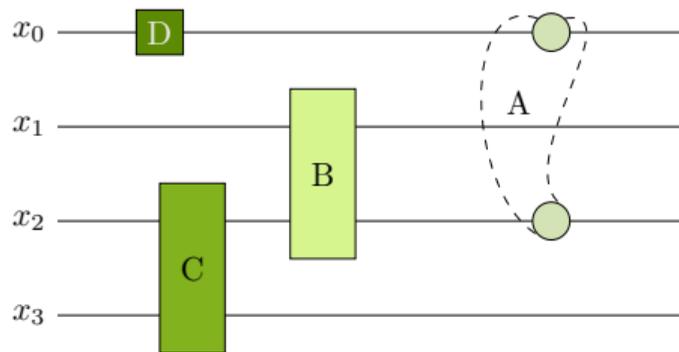


Operators here as before, inputs  $a$  and  $b$ , expression  $b + a(a - \sqrt{a})$ . The 20 character AST string **+b\*a-aQababbabbabab** has a **coding region** (the first 8) shown pictorially as an AST. The last 12 are **non coding**. [Ferreira, 2006]

# Quantum Circuits in GEP

Example of a 4-bit quantum circuit [Alvarez et al., 2023]

QC Practitioner's representation



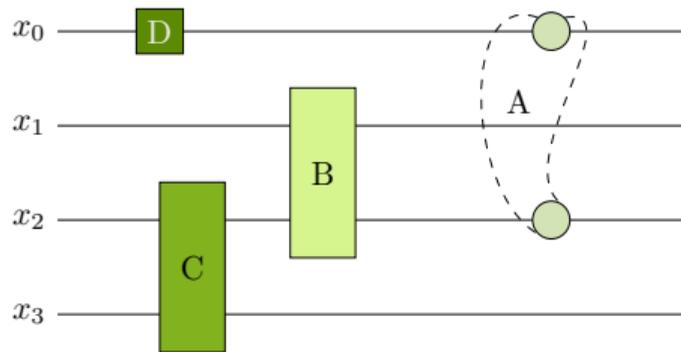
Every gate takes one **input** and produces one **output**

The final output is  $A_{0,2}B_{1,2}C_{2,3}D_0\psi_0$

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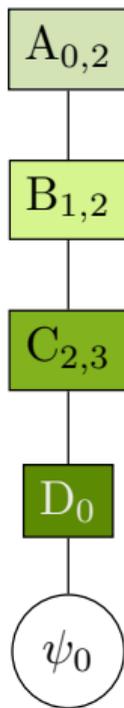
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The QuantumGEP tree



String in GEP  
 $A_{0,2}B_{1,2}C_{2,3}D_0\psi_0$

## QuantumGEP: The Main Algorithm

1. **Start** with an original population of  $M$  circuits generated **randomly**
2. By gene expression programming **mutate** and **combine** the **existing** size  $M$  population, to generate  $M' = 2M$  **new circuits**  $\{\mathcal{C}(\varphi)\}_{0 \leq j < M'}$ <sup>1</sup>

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<sup>1</sup>These circuits may depend on  $K$  continuous variables  $\varphi \equiv \{\varphi_k\}_{0 \leq k < K}$ . For example, consider that the rotation gate may depend on the angle of rotation, and, in general, gates may depend on arbitrary parameters collectively called  $\varphi$ . [Alvarez et al., 2023]

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4. For every circuit  $j$ , **compute the pre-fitness** function  $P_j(\varphi) = -\langle\psi_j(\varphi)|H|\psi_j(\varphi)\rangle$  and find the  $\varphi$  where the maximum occurs; let's call it  $\varphi_{\max}$ .
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5. For every circuit  $j$ , **calculate its fitness**  $F_j \equiv P_j(\varphi_{\max})$ .
6. **Eliminate** the  $M$  circuits with **least fitness** and keep the remaining  $M$  for the next step.
7. **Go to** step 2.

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## Mutations may create wrong trees

Here the string is  $+b^*a-aQa$  and

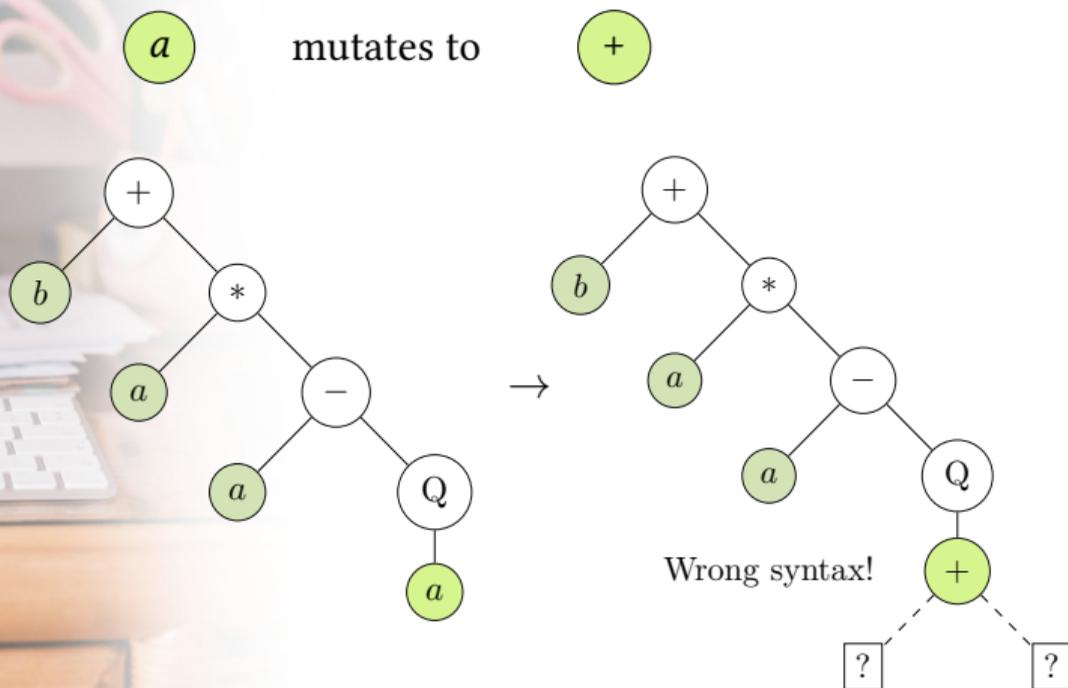


Photo by Sincerely Media

<https://unsplash.com/photos/09K5vvTurCY>

## GEP: Unrestricted Mutations

✂ String has fixed size, with a maximum size **head**. The tail contains only leaves.  
[Ferreira, 2001]  
Yet the **coding section** size varies.

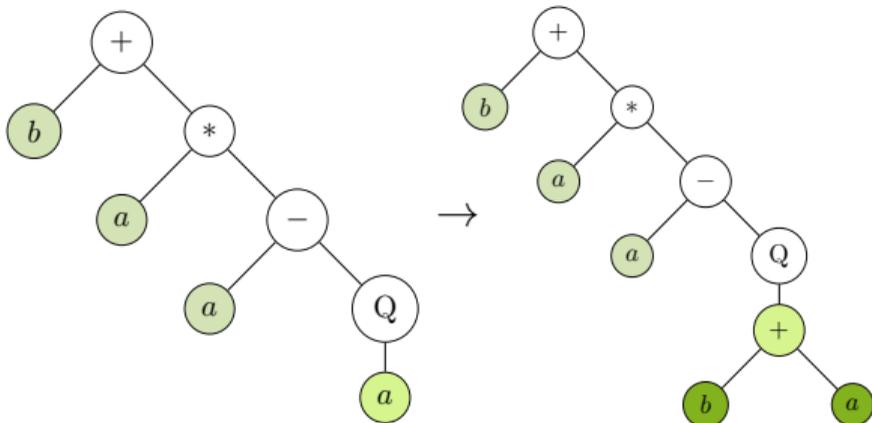
✂ Example. Total Size = 20, Head Max Size=15, and **+b\*a-aQababbabbabab** has 8 coding characters.  
**+b\*a-aQ+babbabbabab** has 10 coding characters.

✂ Mutations **preserve** the head and tail **structure**  
Here **a** **mutates** to **+**

The syntax is still correct thanks to “**junk DNA.**”

**+b\*a-aQababbabbabab** →

**+b\*a-aQ+babbabbabab**



## Results in Condensed Matter

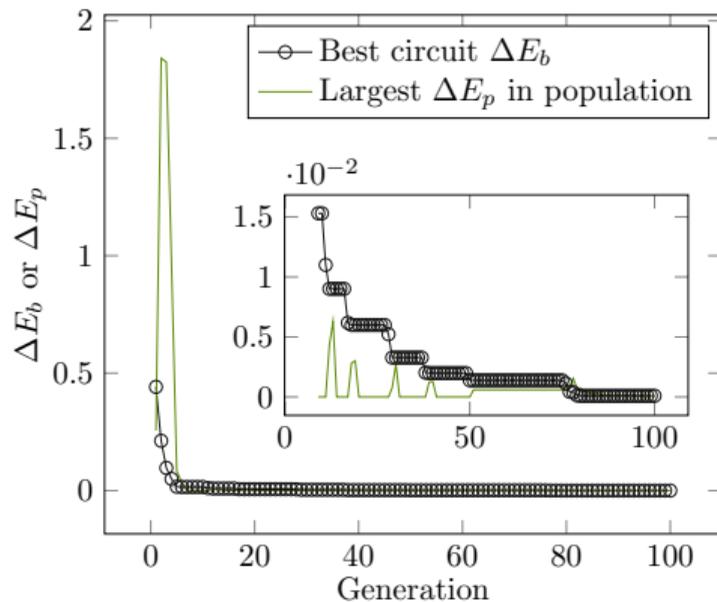
$H = J_x \sum_i \sigma_i^x \sigma_{i+1}^x$ ,  $\sigma^x$  is the Pauli x matrix

Aim: Finding the quantum circuit that produces the **ground state** of  $H$  from  $|0000\rangle$

After a few generations we get many **perfect quantum circuits**

For example, with fitness **3.9971(6)** we find:

$Ry_0:3\pi/2$   $Ry_1:\pi/2$   $Ry_2:3\pi/2$   $Ry_3:\pi/2$



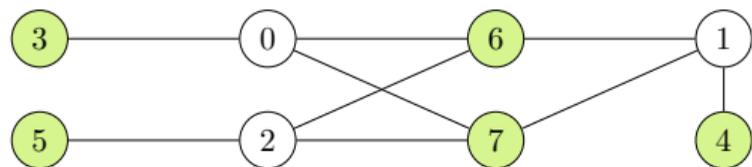
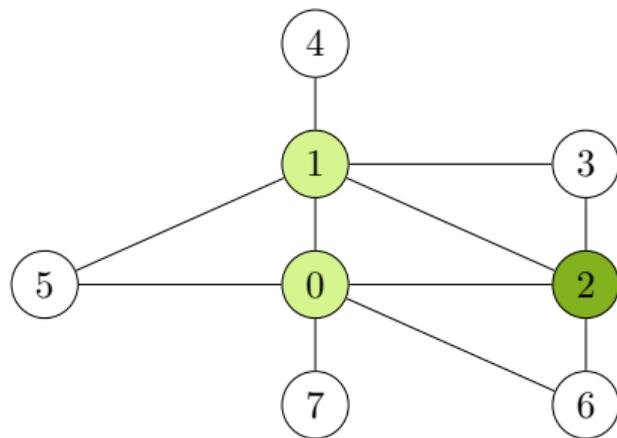
<sup>1</sup>Green line: energy difference between the ground state and that yielded by the best individual at that generation; open circles: largest energy difference within the population at that generation. Inset: magnification of the figure starting at generation eight. [Alvarez et al., 2023]

# Input And Output

```
##Ainur1.0
#This tests GroundState for the XX model on a chain
HeadSize=4;
Population=60;
Generations=20;
NumberOfBits=4;
MinimizerTolerance=0.1;
Primitives="Ry,P";
MinimizerAlgorithm="Simplex";
RunType="GroundState";
Hamiltonian="xx";
HamiltonianCoupling=1;
#HamiltonianIsPeriodic=1;
InVectorFile="../../TestSuite/inputs/vector10.txt";

./quantumGep -f ../../TestSuite/inputs/input10.ain
Ground State Energy=-3
Ry2:4.445622188 Ry0:0.4704532758 Ry1:1.806751358 Ry0:6.017431122 0 fit 1.43069 0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100 101 102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 139 140 141 142 143 144 145 146 147 148 149 150 151 152 153 154 155 156 157 158 159 160 161 162 163 164 165 166 167 168 169 170 171 172 173 174 175 176 177 178 179 180 181 182 183 184 185 186 187 188 189 190 191 192 193 194 195 196 197 198 199 200 201 202 203 204 205 206 207 208 209 210 211 212 213 214 215 216 217 218 219 220 221 222 223 224 225 226 227 228 229 230 231 232 233 234 235 236 237 238 239 240 241 242 243 244 245 246 247 248 249 250 251 252 253 254 255 256 257 258 259 260 261 262 263 264 265 266 267 268 269 270 271 272 273 274 275 276 277 278 279 280 281 282 283 284 285 286 287 288 289 290 291 292 293 294 295 296 297 298 299 300 301 302 303 304 305 306 307 308 309 310 311 312 313 314 315 316 317 318 319 320 321 322 323 324 325 326 327 328 329 330 331 332 333 334 335 336 337 338 339 340 341 342 343 344 345 346 347 348 349 350 351 352 353 354 355 356 357 358 359 360 361 362 363 364 365 366 367 368 369 370 371 372 373 374 375 376 377 378 379 380 381 382 383 384 385 386 387 388 389 390 391 392 393 394 395 396 397 398 399 400 401 402 403 404 405 406 407 408 409 410 411 412 413 414 415 416 417 418 419 420 421 422 423 424 425 426 427 428 429 430 431 432 433 434 435 436 437 438 439 440 441 442 443 444 445 446 447 448 449 450 451 452 453 454 455 456 457 458 459 460 461 462 463 464 465 466 467 468 469 470 471 472 473 474 475 476 477 478 479 480 481 482 483 484 485 486 487 488 489 490 491 492 493 494 495 496 497 498 499 500 501 502 503 504 505 506 507 508 509 510 511 512 513 514 515 516 517 518 519 520 521 522 523 524 525 526 527 528 529 530 531 532 533 534 535 536 537 538 539 540 541 542 543 544 545 546 547 548 549 550 551 552 553 554 555 556 557 558 559 560 561 562 563 564 565 566 567 568 569 570 571 572 573 574 575 576 577 578 579 580 581 582 583 584 585 586 587 588 589 590 591 592 593 594 595 596 597 598 599 600 601 602 603 604 605 606 607 608 609 610 611 612 613 614 615 616 617 618 619 620 621 622 623 624 625 626 627 628 629 630 631 632 633 634 635 636 637 638 639 640 641 642 643 644 645 646 647 648 649 650 651 652 653 654 655 656 657 658 659 660 661 662 663 664 665 666 667 668 669 670 671 672 673 674 675 676 677 678 679 680 681 682 683 684 685 686 687 688 689 690 691 692 693 694 695 696 697 698 699 700 701 702 703 704 705 706 707 708 709 710 711 712 713 714 715 716 717 718 719 720 721 722 723 724 725 726 727 728 729 730 731 732 733 734 735 736 737 738 739 740 741 742 743 744 745 746 747 748 749 750 751 752 753 754 755 756 757 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2006 2007 2008 2009 2010 2011 2012 2013 2014 2015 2016 2017 2018 2019 2020 2021 2022 2023 2024 2025 2026 2027 2028 2029 2030 2031 2032 2033 2034 2035 2036 2037 2038 2039 2040 2041 2042 2043 2044 2045 2046 2047 2048 2049 2050 2051 2052 2053 2054 2055 2056 2057 2058 2059 2060 2061 2062 2063 2064 2065 2066 2067 2068 2069 2070 2071 2072 2073 2074 2075 2076 2077 2078 2079 2080 2081 2082 2083 2084 2085 2086 2087 2088 2089 2090 2091 2092 2093 2094 2095 2096 2097 2098 2099 2100 2101 2102 2103 2104 2105 2106 2107 2108 2109 2110 2111 2112 2113 2114 2115 2116 2117 2118 2119 2120 2121 2122 2123 2124 2125 2126 2127 2128 2129 2130 2131 2132 2133 2134 2135 2136 2137 2138 2139 2140 2141 2142 2143 2144 2145 2146 2147 2148 2149 2150 2151 2152 2153 2154 2155 2156 2157 2158 2159 2160 2161 2162 2163 2164 2165 2166 2167 2168 2169 2170 2171 2172 2173 2174 2175 2176 2177 2178 2179 2180 2181 2182 2183 2184 2185 2186 2187 2188 2189 2190 2191 2192 2193 2194 2195 2196 2197 2198 2199 2200 2201 2202 2203 2204 2205 2206 2207 2208 2209 2210 2211 2212 2213 2214 2215 2216 2217 2218 2219 2220 2221 2222 2223 2224 2225 2226 2227 2228 2229 2230 2231 2232 2233 2234 2235 2236 2237 2238 2239 2240 2241 2242 2243 2244 2245 2246 2247 2248 2249 2250 2251 2252 2253 2254 2255 2256 2257 2258 2259 2260 2261 2262 2263 2264 2265 2266 2267 2268 2269 2270 2271 2272 2273 2274 2275 2276 2277 2278 2279 2280 2281 2282 2283 2284 2285 2286 2287 2288 2289 2290 2291 2292 2293 2294 2295 2296 2297 2298 2299 2300 2301 2302 2303 2304 2305 2306 2307 2308 2309 2310 2311 2312 2313 2314 2315 2316 2317 2318 2319 2320 2321 2322 2323 2324 2325 2326 2327 2328 2329 2330 2331 2332 2333 2334 2335 2336 2337 2338 2339 2340 2341 2342 2343 2344 2345 2346 2347 2348 2349 2350 2351 2352 2353 2354 2355 2356 2357 2358 2359 2360 2361 2362 2363 2364 2365 2366 2367 2368 2369 2370 2371 2372 2373 2374 2375 2376 2377 2378 2379 2380 2381 2382 2383 2384 2385 2386 2387 2388 2389 2390 2391 2392 2393 2394 2395 2396 2397 2398 2399 2400 2401 2402 2403 2404 2405 2406 2407 2408 2409 2410 2411 2412 2413 2414 2415 2416 2417 2418 2419 2420 2421 2422 2423 2424 2425 2426 2427 2428 2429 2430 2431 2432 2433 2434 2435 2436 2437 2438 2439 2440 2441 2442 2443 2444 2445 2446 2447 2448 2449 2450 2451 2452 2453 2454 2455 2456 2457 2458 2459 2460 2461 2462 2463 2464 2465 2466 2467 2468 2469 2470 2471 2472 2473 2474 2475 2476 2477 2478 2479 2480 2481 2482 2483 2484 2485 2486 2487 2488 2489 2490 2491 2492 2493 2494 2495 2496 2497 2498 2499 2500 2501 2502 2503 2504 2505 2506 2507 2508 2509 2510 2511 2512 2513 2514 2515 2516 2517 2518 2519 2520 2521 2522 2523 2524 2525 2526 2527 2528 2529 2530 2531 2532 2533 2534 2535 2536 2537 2538 2539 2540 2541 2542 2543 2544 2545 2546 2547 2548 2549 2550 2551 2552 2553 2554 2555 2556 2557 2558 2559 2560 2561 2562 2563 2564 2565 2566 2567 2568 2569 2570 2571 2572 2573 2574 2575 2576 2577 2578 2579 2580 2581 2582 2583 2584 2585 2586 2587 2588 2589 2590 2591 2592 2593 2594 2595 2596 2597 2598 2599 2600 2601 2602 2603 2604 2605 2606 2607 2608 2609 2610 2611 2612 2613 2614 2615 2616 2617 2618 2619 2620 2621 2622 2623 2624 2625 2626 2627 2628 2629 2630 2631 2632 2633 2634 2635 2636 2637 2638 2639 2640 2641 2642
```

## Results for the Max-Cut Problem



A **solution** is given by 248, (binary) 11111000: sites 3 to 7 have down spins and form the maximal cut; **energy equals -9**, fitness 9.

A **solution** is given by 3 or 7. The number, 3, is binary 00000011: sites 0, 1, have down spins and form the maximal cut; The other solution is 7, (binary) 00000111: sites 0, 1, and 2 form the maximal cut. Vertices 0, 1, and 2 have been shaded, with vertex 2 shaded more to indicate that it appears only in the 2nd solution. In all cases **energy is -5**, fitness 5.<sup>2</sup>

<sup>2</sup>Both graphs in [Alvarez et al., 2023] appear also in [Lotshaw et al., 2021]

## Advanced Features in GEP

*(1) Multiple genes*

*(2) Numerical constants*

---

<sup>2</sup>Adapted from Figures 5.2 and 3.13 in [Ferreira, 2006].

# Advanced Features in GEP

## (1) Multiple genes

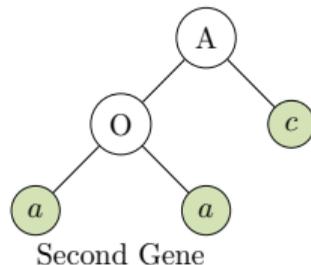
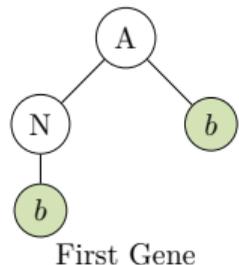
## (2) Numerical constants

Logical primitives: {And, Not, Or}

Leaves: {a, b, c};  $a, b, c \in \{\text{true}, \text{false}\}$

01234560123456

ANbbabcAOcaabc



---

<sup>2</sup>Adapted from Figures 5.2 and 3.13 in [Ferreira, 2006].

# Advanced Features in GEP

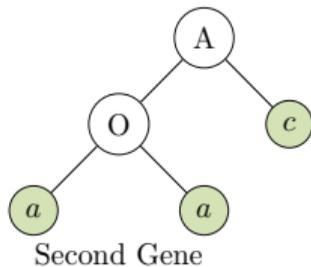
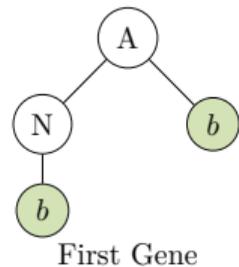
## (1) Multiple genes

Logical primitives: {And, Not, Or}

Leaves: {a, b, c}; a,b,c ∈ {true, false}

01234560123456

ANbbabcAOcaabc



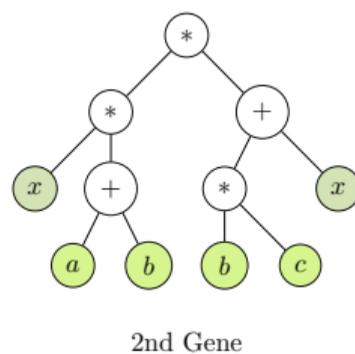
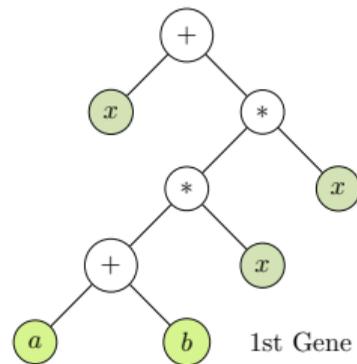
## (2) Numerical constants

Primitives: arithm. set; leaf: x

Constants: a=0.298, b=1.083, c=1.466

01234567890120123456789012

+x\*x+xabbcae\*x\*x+x\*xabbcae



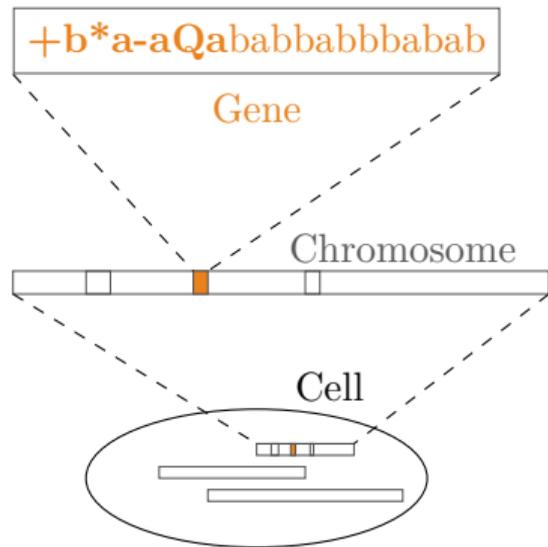
<sup>2</sup>Adapted from Figures 5.2 and 3.13 in [Ferreira, 2006].

# Automatically Defined Functions

✂ **Multiple genes** form a chromosome  
*And multiple **chromosomes** form a cell*

✂ **A cell** may produce multiple outputs,  
*Or may be controlled by **a single output***

✂ **ADFs** then create a hierarchy



# Summary and Outlook

## QuantumGEP...

✧ **yields** thousands of quantum circuits for each problem  
*And they aren't parametric*

✧ **shows** success in condensed matter and graph theory  
*And may work in other domain sciences; [arxiv.2303.08203](https://arxiv.org/abs/2303.08203)*

✧ **has** a free and open source license  
*And development happens in the open*

[code.ornl.gov/gonzalo\\_3/evendim](https://code.ornl.gov/gonzalo_3/evendim)  
[github.com/g1257/evendim](https://github.com/g1257/evendim)



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Tikz was used for some figures.

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