As the complexity of quantum systems such as quantum bit arrays increases, efforts to automate expensive tuning are increasingly worthwhile. We investigate machine learning based tuning of gate arrays using the CMA-ES algorithm for the case study of Majorana wires with strong disorder. We find that the algorithm is able to efficiently improve the topological signatures, learn intrinsic disorder profiles, and completely eliminate disorder effects. For example, with only 20 gates, it is possible to fully recover Majorana zero modes destroyed by disorder by optimizing gate voltages.

Setup: A schematic of the Majorana hybrid wire embedded into one arm of an Aharonov-Bohm interferometer is shown in Fig. 1. Our goal is to find voltages $V_g$ of $N_g$ gates of the Majorana wire as a metric, which can be measured by placing the wire in an arm of an electron interferometer [81] and allows to distinguish MZMs from ABSs [80, 82].

Machine learning optimization of Majorana hybrid nanowires

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Introduction: In recent years, increasingly complex quantum devices such as quantum bit arrays have been proposed and implemented [1–5], requiring more personnel-intensive tuning. Therefore, it is becoming profitable, and in some cases even necessary, to automate the tuning process [6–8], and machine learning approaches have been found to be very flexible and robust for this purpose [5, 7–12]. Especially for the implementation of large scale quantum computation [13–16], efficient tuning of parameters and gates is crucial and numerous automations in quantum dot based qubits have been proposed [6–8, 10, 11, 17–23].

A popular platform for scalable qubit architectures is based on Majorana zero modes (MZMs) in topological superconductors [1, 4, 24–29], whose advantages are the non-local storage of quantum information and its manipulation via anyonic braiding [24–27, 30]. MZMs have been proposed to exist in semiconductor-superconductor heterostructures [24, 31–34] and many of their predicted signatures have been observed, such as zero-bias conductance peaks [35–38], the fractional Josephson effect [39], and the suppression of even-odd splitting difference of conductance resonances in Coulomb blockade [40]. For a clean wire, it has been theoretically demonstrated that a harmonic potential profile [41] and specially chosen magnetic field textures [41–44] can make MZMs more robust, and the geometry of Majorana Josephson junctions has been optimized to increase the size of the topological gap [45]. Nevertheless, disorder remains a crucial problem [46–49] in such systems, as it can mimic MZM signatures even in the topologically trivial region [46, 48, 50–53], or destroy the topological phase altogether [54].

In this letter, we present a case study of automatic tuning of a gate array in proximity to a strongly disordered Majorana wire using the CMA-ES algorithm [55, 56] which maximizes the amplitude $A$ of coherent transmission through a Majorana hybrid wire embedded into one arm of an Aharonov-Bohm interferometer. Initially, one sets a step size $\sigma^{(0)}$, a covariance matrix $C^{(0)}$, and starting gate voltages $V_g^{(0)}$. In each iteration $t$, $n$ gate voltage configurations are drawn from a multivariate normal distribution with mean $V_g^{(t)}$ and covariance $C^{(t)}$. Based on the amplitudes $A_i$ for the proposed gate voltage configurations $V_g^{(t)}$, the new mean value $V_g^{(t+1)}$ is determined, and step size $\sigma^{(t+1)}$ and covariance $C^{(t+1)}$ are updated.

![Figure 1. Schematic diagram of the Covariance Matrix Adaptation Evolution Strategy (CMA-ES) algorithm.](cond-mat.mes-hall)
We first consider a strictly one-dimension model for the hybrid wire, and generalize to a more realistic two-dimensional model later. The Majorana wire consisting of a semiconductor with Rashba spin-orbit coupling $\alpha_R$ and a proximity induced s-wave gap $\Delta$ is described in the Nambu basis $\left(d_\uparrow(y), d_\downarrow(y), d_\downarrow(y), -d_\uparrow(y)\right)$ by the Hamiltonian
\begin{equation}
\mathcal{H}_{\text{wire}} = \tau_z \left[ -\frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial y^2} \sigma_0 - \mu \sigma_0 - i\hbar \alpha_R \sigma_x \partial_y \right. \\
+ \delta_{\text{dis}}(y) \sigma_0 + V_g(y) \sigma_0 + V_{\text{conf}}(y) \sigma_0 \right] - E_z \tau_0 \sigma_z + \Delta \tau_x \sigma_0 ,
\end{equation}
with disorder potential $\delta_{\text{dis}}$, confinement potential $V_{\text{conf}}$, gate potential $V_g$ (see Eq. (2)), and Pauli matrices $\sigma_i$ and $\tau_z$ acting in spin and particle-hole space, respectively. Rashba spin-orbit coupling defines a characteristic energy scale $E_{\text{so}} = \alpha_R^2 m^*/2 = 0.05 \text{ meV}$ and length scale $l_{\text{so}} = \hbar/(\alpha_R m^*) = 0.19 \text{ nm}$ of the system, where $\hbar = 0.2 eV \AA$ and $m^* = 0.02 m_e$ are realistic values for InAs [29, 35]. Throughout this paper, we consider wires of length $L = 13 l_{\text{so}}$ on a grid with spacing $a = 0.026 l_{\text{so}}$.

We use a chemical potential $\mu = 1 E_{\text{so}}$, a Zeeman energy $E_z = 6 E_{\text{so}}$, and gap $\Delta = 2 E_{\text{so}}$, such that the system in the absence of disorder and gate voltages is in the topological regime.

We describe disorder in the wire by first drawing random numbers $\delta$ with standard deviation $\sigma_{\text{dis}}$ from a normal distribution and then introduce a finite correlation length $\lambda_{\text{dis}}$ by damping high Fourier modes according to
\begin{equation}
\delta_{\text{dis}}(y) = \mathcal{F}^{-1} \left[ e^{-|q| \lambda_{\text{dis}}^2} \mathcal{F} \left[ \delta(y) \right] \right] .
\end{equation}
Here the case $\lambda_{\text{dis}} = 0$ corresponds to onsite disorder.

Wire and leads are connected via deep tunnel barriers of shape $V_{\sigma}(y) = V_0 \exp[-y^2/(2\sigma^2)]$ with $\sigma = 0.1 l_{\text{so}}$ and $V_0 = 65 E_{\text{so}}$, which we assume to be defined by separate gates that are not included in the optimization. For simplicity, we assume that the leads are normal conducting and without spin orbit coupling. We treat Coulomb blockade in the Majorana wire using a mean-field approximation, such that adding an electron to the system of $N_0$ electrons costs an additional charging energy $E_c = 8 E_{\text{so}}$, and introduce effective energy levels $\varepsilon_{\text{eff},j}$ containing both charging energy and single particle energies. We consider the system to be tuned to the center between the conductance resonances for a fixed particle number $N_0$ in the Majorana wire.

Finally, using the Weidenmüller formula [83]
\begin{equation}
T = i \varphi_R \Gamma_R U_w \frac{1}{\varepsilon - \text{diag} (\varepsilon_{\text{eff}}) - U_w \Sigma U_w} U_w^\dagger \Gamma_L \varphi_L ,
\end{equation}
with eigenvectors $U_w$ of the wire Hamiltonian Eq. (3), we can determine the transmission amplitude $A = |T_{\uparrow\uparrow} + T_{\downarrow\downarrow}|$.
in the middle between conductance resonances. Here, $\varepsilon$ is the energy of incoming electrons in the lead, and self-energies $\Sigma_{\alpha}$, $\Gamma_{\alpha} = i(\Sigma_{\alpha} - \Sigma_{\alpha}^\dagger)$, $\Sigma = \sum_{\alpha} \Sigma_{\alpha}$, and propagating modes $\varphi_{\alpha}$ of lead $\alpha$ are obtained by using the Python package KWANT [84].

A finite temperature can be considered by computing the scattering matrix for different thermal excitations of the wire and thermally averaging the transmission amplitude. Then, the transmission amplitude vanishes in the case of trivial ABSs [80, 82], such that our metric is able to distinguish true MZM from an ABS. For the optimization, we consider transport through the first 10 levels and verify the final results by taking into account 50 levels. We carefully checked that this does not influence the optimization results.

In the absence of disorder and with zero voltage at all gates, the lowest level of the wire is approximately at zero energy in the middle of the topological gap (see Fig. 2c), and the associated wave function $\Psi_0 = (u_0, v_0)$ is localized at the wire ends and satisfies the Majorana condition $|u_0(y)| = |v_0(y)|$ (Fig. 2a). However, if one adds strong disorder (Fig. 2d), both topological gap (red circles, Fig. 2c) and MZMs (Fig. 2b) are destroyed. As a result, the associated transmission amplitude is reduced by two orders of magnitude as compared to the clean wire. 

**Optimization results:** To understand the convergence behavior and the influence of the population size $n_{\text{pop}}$ on the CMA-ES algorithm, we consider two scenarios: (i) disorder with a finite correlation length $\lambda_{\text{dis}} = 0.052 l_0$ and (ii) onsite disorder. For both cases, we perform a CMA-ES optimization of 20 gates with population sizes $n_{\text{pop}} = 12$ and $n_{\text{pop}} = 80$. In the easier case (i) already the smaller population size is sufficient to achieve fast convergence after less than 1000 function evaluations (brown line Fig. 3a), whereas for $n_{\text{pop}} = 80$ about five times as many evaluations are necessary (brown line Fig. 3b). In contrast, we find that the more difficult problem (ii) converges poorly in the case of small population sizes, but converges almost as fast as the correlated disorder case for $n_{\text{pop}} = 80$. Thus, if the primary time effort is to perform a function evaluation, i.e., a measurement of the metric in the experiment, we recommend to deviate from the standard value $n_{\text{pop}} = 4 + 3 \ln(N_\text{g} - 1)$ [85] for the case of a small disorder correlation length.

We distinguish between two different types of optimizations in the following: (i) optimization in the absence of disorder to determine what shape a potential should have to improve the localization properties of the MZMs ("wave function engineering"), and (ii) optimization with disorder in the wire. In the case of wave function engineering for 20 gates, we find an enhancement of the transmission amplitude by a factor of about 1.6 by optimizing the localization of the MZMs (Fig. 4a) while keeping a sizable topological gap (inset). To achieve this, potentials of the outermost gates are lowered to draw more weight of the wave functions to the wire ends (Fig. 4c, [86]). In case (ii) with disorder (c.f. Fig. 2b), the optimization almost completely restores the MZMs and the topological gap, increasing the transmission amplitude by two orders of magnitude (Fig. 4b).
average disorder (dashed red line Fig. 4d), in addition to the zero disorder optimal values (Fig. 4d). We emphasize that the CMA-ES algorithm has no knowledge about system parameters, but only suggests gate configurations based on corresponding transmission amplitudes.

Having seen from the examples how optimization can make MZMs more robust, we next consider how reliable the optimization is for different disorder correlation lengths, how many gates are necessary, and how strong the dependence on the seed of the CMA-ES random number generator is. For this, we consider 15 different values for the number of gates, from \( N_g = 4 \) to \( N_g = 200 \), and three types of disorder, onsite \( (\lambda_{\text{dis}} = 0) \), \( \lambda_{\text{dis}} = 0.052 l_{\text{so}} \) and \( \lambda_{\text{dis}} = 0.052 l_{\text{so}} \), as well as wave function engineering without disorder. For the case with disorder, we consider ten different disorder realizations and average the resulting amplitudes, while in the absence of disorder we average over ten different seeds of the CMA-ES algorithm. We find that for at least 20 gates all considered disorder profiles can be compensated reliably (see Fig. 5). For too few gates \( N_g \leq 10 \), it is no longer possible to remove disorder with very small correlation length. For many gates, \( N_g \approx 100 \), the amplitude saturates, having increased by one order of magnitude as compared to \( N_g = 20 \), but with the drawback that up to \( 10^5 \) function evaluations are needed to achieve full convergence. We observe a sweet spot \( 20 \leq N_g \leq 50 \), where the number of necessary function evaluations is acceptable and still significant improvements of the amplitude and complete compensation of disorder are possible.

Choice of metric: Above, we have chosen the coherent transmission amplitude, since it distinguishes ABS from MZMs [80, 82] and benefits from enhanced localization of MZMs. For a Majorana wire, other metrics come to mind that may be easier to determine experimentally, which however turn out to cause problems in the optimization process. For example, optimizing the gap \(|\varepsilon_1 - \varepsilon_0|\) has the disadvantage that it does not require \( \varepsilon_0 \) to be small and in addition does not depend on the localization at the wire ends. On the other hand, when minimizing the lowest level \( \varepsilon_0 \), localization of MZMs is not strengthened, and in addition one is not able to exclude a vanishing gap or the presence of ABSs. Optimizing the incoherent part of the conductance through the wire produces trivial ABSs instead of MZMs by lowering the outermost gates [86] to create potential wells at the ends [68], while increasing the effective chemical potential in the remaining wire, thus lifting it into the trivial regime.

Two dimensional case: We study a wire with length \( L_y = 13 l_{\text{so}} \) and width \( L_x = 0.39 l_{\text{so}} \), and account for the orbital effect of the magnetic field by adding Peierls phases \( e^{-ie/c} \int r_1 \varphi^2 A \cdot dr \) to the hoppings from site \( r_1 \) to site...
We choose a chemical potential $\mu = 63 \, E_{so}$ and Zeeman energy $E_z = 6 \, E_{so}$, such that the wire in the absence of disorder and gates is in the topological regime with one occupied subband (a discussion of transport through higher subbands can be found in [86]). In the presence of strong disorder, the MZMs are destroyed (Fig. 6a) and the gap collapses (red circles in Fig. 6d), but again optimization with only 20 gates along the wire can restore the gap (blue crosses in Fig. 6d) as well as the gap (blue crosses in Fig. 6d) similar to the one dimensional case.

Conclusions: We studied machine learning optimization of a gate array using the CMA-ES algorithm. Using the coherent transmission amplitude through a Coulomb blocked Majorana wire as metric, we find: (i) optimization in absence of disorder improves localization of MZMs significantly and (ii) optimization even restores MZMs fully in the case of strong disorder that otherwise destroys the topological phase. We discussed the importance of the choice of an appropriate metric, showed that the number of necessary function evaluations would be experimentally feasible, and that a moderate number of gates is sufficient for restoration of MZMs in the presence of disorder.

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[1] T. Karzig, C. Knapp, R. M. Lutchyn, P. Bonder son, M. B. Hastings, C. Nayak, J. Alicea, K. Flens berg, S. Plugge, Y. Oreg, C. M. Marcus, and M. H. Freedman, Scalable designs for quasiparticle-poisoning-protected topological quantum computation with Majorana zero modes, Physical Review B 95, 235305 (2017).

[2] F. Arute, K. Arya, R. Babbush, D. Bacon, J. C. Bardin, R. Barends, R. Biswas, S. Boixo, Brandao, Fernando G. S. L., D. A. Buell, B. Burkett, Y. Chen, Z. Chen, B. Chiaro, R. Collins, W. Courtney, A. Dunsworth, E. Farhi, B. Foxen, A. Fowler, C. Gidney, M.Giustina, R. Graff, K. Grauer, S. Habegger, M. P. Harrigan, M. J. Hartmann, A. Ho, M. Hoffmann, T. Huang, T. S. Humble, S. V. Isakov, E. Jeffrey, Z. Jiang, D. Kafri, K. Kechedzhi, J. Kelly, P. V. Klimov, S. Knysz, A. Korotkov, F. Kostritsa, D. Landhuis, M. Lindmark, E. Lucero, D. Lyakh, S. Mandrà, J. R. McClean, M. McEwen, A. Megrant, X. Mi, K. Michielsen, M. Mohseni, J. Mutus, O. Naaman, M. Neely, C. Neill, M. Y. Niu, E. Ostby, A. Petukhov, J. C. Platt, C. Quintana, E. G. Rieffel, P. Roushan, N. C. Rubin, D. Sank, K. J. Satzinger, V. Smelyanskiy, K. J. Sung, M. D. Trottibich, A. Vainsencher, B. Villalonga, T. White, Z. J. Yao, P. Yeh, A. Zalcman, H. Neven, and J. M. Martinis, Quantum supremacy using a programmable superconducting processor, Nature 574, 505 (2019).

[3] D. T. Lennon, H. Moon, L. C. Camenzind, L. Yu, D. M. Zumbibl, G. A. D. Briggs, M. A. Osborne, E. A. Laird, and N. Ares, Efficiently measuring a quantum device using machine learning, npj Quantum Information 5, 1 (2019).

[4] Y. Oreg and F. von Oppen, Majorana Zero Modes in Networks of Cooper-Pair Boxes: Topologically Ordered States and Topological Quantum Computation, Annual Review of Condensed Matter Physics 11, 397 (2020).

[5] N. Ares, Machine learning as an enabler of qubit scalability, Nature Reviews Materials 6, 870 (2021).

[6] T. A. Baart, P. T. Eendebak, C. Reichl, W. Wegscheider, and L. M. K. Vandersypen, Computer-automated tuning of semiconductor double quantum dots into the single-electron regime, Applied Physics Letters 108, 213104 (2016).

[7] D. L. Craig, H. Moon, F. Fedele, D. T. Lennon, B. van Straaten, F. Vignue, L. C. Camenzind, D. M. Zumbibl, G. A. D. Briggs, M. A. Osborne, D. Sejidinovic, and N. Ares, Bridging the reality gap in quantum devices with physics-aware machine learning.

[8] J. Ziegler, T. McJunkin, E. S. Joseph, S. S. Kalantre, B. Harpt, D. E. Savage, M. G. Lagally, M. A. Eriksson, J. M. Taylor, and J. P. Zwolak, Toward Robust Autotuning of Noisy Quantum Dot Devices.

[9] A. Fries, J. K. Gamble, D. R. Ward, R. Blume-Kohout, M. A. Eriksson, M. Friesen, and S. N. Coppersmith, Compressed Optimization of Device Architectures for Semiconductor Quantum Devices, Physical Review Applied 11, 024063 (2019).

[10] S. S. Kalantre, J. P. Zwolak, S. Ragole, X. Wu, N. M. Zimmerman, M. D. Stewart, and J. M. Taylor, Machine learning techniques for state recognition and auto-tuning in quantum dots, npj Quantum Information 5, 1 (2019).

[11] H. Moon, D. T. Lennon, J. Kirkpatrick, N. M. van Esbroeck, L. C. Camenzind, L. Yu, F. Vignue, D. M. Zumbibl, G. A. D. Briggs, M. A. Osborne, D. Sejidinovic, E. A. Laird, and N. Ares, Machine learning enables completely automatic tuning of a quantum device faster than human experts, Nature Communications 11, 4160 (2020).

[12] H.-C. Ruiz Euler, M. N. Boon, J. T. Wildeboer, B. van de Ven, T. Chen, H. Broersma, P. A. Bobbert, and W. G. van der Wiel, A deep-learning approach to realizing functionality in nano-electronic devices, Nature Nanotechnology 15, 992 (2020).

[13] T. D. Ladd, F. Jelezko, R. Laflamme, Y. Nakamura, C. Monroe, and J. L. O’Brien, Quantum computers, Nature 464, 45 (2010).

[14] R. Hanson, L. P. Kouwenhoven, J. R. Petta, S. Tarucha, and L. M. K. Vandersypen, Spins in few-electron quantum dots, Reviews of Modern Physics 79, 1217 (2007).

[15] C. Kloeffel, D. Z. O. and D. Loss, Prospects for Spin-Based Quantum Computing in Quantum Dots, Annual Review of Condensed Matter Physics 4, 51 (2013).

[16] M. J. K. Vandersypen, H. Blium, J. S. Clarke, A. S. Dzurak, R. Ishihara, A. Morello, D. J. Reilly, L. R. Schreiber, and M. Veldhorst, Interfacing spin qubits in quantum arrays, npj Quantum Information 3, 1 (2017).

[17] T. Botzem, M. D. Shulman, S. Foletti, S. P. Harvey, O. E. Dial, P. Bethke, P. Cerfontaine, R. P. G. McNeil, D. Mahalu, V. Umansky, A. Ludwig, A. Wieck, D. Schuh, D. Bougeard, A. Yakoby, and H. Blium, Tuning Methods...
[18] J. D. Teske, S. S. Humphol, R. Otten, P. Bethke, P. Cerfontaine, J. Dedden, A. Ludwig, A. D. Wieck, and H. Bluhm, A machine learning approach for automated fine-tuning of semiconductor spin qubits, Applied Physics Letters 114, 133102 (2019).

[19] A. R. Mills, M. M. Feldman, C. Monical, P. J. Lewis, K. W. Larson, A. M. Mounce, and J. R. Petta, Computer-automated tuning procedures for semiconductor quantum dot arrays, Applied Physics Letters 115, 113501 (2019).

[20] R. Durrer, B. Kratochwil, J. V. Koski, A. J. Landig, C. Reichl, W. Wegscheider, T. Ihn, and E. Greplova, Automated Tuning of Double Quantum Dots into Specific Charge States Using Neural Networks, Physical Review Applied 13, 054019 (2020).

[21] N. M. van Esbroeck, D. T. Lennon, H. Moon, V. Nguyen, F. Vignéau, L. C. Camenzind, L. Yu, D. M. Zumbühl, G. A. D. Briggs, D. Sejdinovic, and N. Ares, Quantum device fine-tuning using unsupervised embedding learning, New Journal of Physics 22, 095003 (2020).

[22] F. Fedele, A. Chatterjee, S. Fallahi, G. C. Gardner, M. J. Manfra, and F. Kuemmeth, Simultaneous Operations in a Two-Dimensional Array of Singlet-Triplet Qubits, PRX Quantum 2, 040306 (2021).

[23] O. Krause, A. Chatterjee, F. Kuemmeth, and E. van Nieuwenburg, Learning coulomb diamonds in large quantum dot arrays, arXiv preprint arXiv:2205.01443 (2022).

[24] J. Alicea, Y. Oreg, G. Refael, and F. von Oppen, Helical liquids for Majorana fermions and a topological phase transition in wires, Physics-Uspekhi 94, 177002 (2010).

[25] Y. Oreg, G. Refael, and F. von Oppen, Majorana fermion bound states in quantum wires, Physical review letters 105, 077001 (2010).

[26] Y. Oreg, G. Refael, and F. von Oppen, Helical liquids and Majorana bound states in quantum wires, Physical review letters 105, 177002 (2010).

[27] S. Ahn, H. Pan, B. Woods, T. D. Stanescu, and S. Das Sarma, Estimating disorder and its adverse effects in semiconductor Majorana nanowires, arXiv:2109.00007 (2021).

[28] S. Das Sarma and H. Pan, Disorder-induced zero-bias
peaks in Majorana nanowires, Physical Review B 103, 195158 (2021).

P. Yu, J. Chen, M. Gomanko, G. Badawy, Bakkers, E. P. A. M., K. Zuo, V. Mourik, and S. M. Frolov, Non-Majorana states yield nearly quantized conductance in proximitized nanowires, Nature Physics 17, 482 (2021).

D. Bagrets and A. Altland, Class D spectral peak in Majorana quantum wires, Physical review letters 109, 227005 (2012).

D. I. Pikulin, J. P. Dahlhaus, M. Wimmer, H. Schomerus, and C. W. J. Beenakker, A zero-voltage conductance peak from weak antilocalization in a Majorana nanowire, New Journal of Physics 14, 125011 (2012).

J. Liu, A. C. Potter, K. T. Law, and P. A. Lee, Zero-bias peaks in the tunneling conductance of spin-orbit-coupled superconducting wires with and without Majorana end-states, Physical review letters 109, 267002 (2012).

H. Pan and S. Das Sarma, Physical mechanisms for zero-bias conductance peaks in Majorana nanowires, Physical Review Research 2, 013377 (2020).

S. Takei, B. M. Fregoso, H.-Y. Hui, A. M. Lobos, and S. Das Sarma, Soft superconducting gap in semiconductor Majorana nanowires, Physical review letters 110, 186803 (2013).

N. Hansen and A. Ostermeier, Completely derandomized self-adaptation in evolution strategies, Evolutionary Computation 9, 159 (2001).

N. Hansen, S. D. Müller, and P. Koumoutsakos, Reducing the time complexity of the derandomized evolution strategy with covariance matrix adaptation (CMA-ES), Evolutionary Computation 11, 1 (2003).

N. Hansen, The CMA Evolution Strategy: A Comparing Review, in Towards a New Evolutionary Computation, Studies in Fuzziness and Soft Computing, edited by J. A. Lozano, E. Bengoetxea, I. Inza, and P. Larrañaga (Springer-Verlag Berlin Heidelberg, Berlin, Heidelberg, 2006) pp. 75–102.

J. A. Lozano, E. Bengoetxea, I. Inza, and P. Larrañaga, eds., Towards a New Evolutionary Computation: Advances in the Estimation of Distribution Algorithms, Studies in Fuzziness and Soft Computing, Vol. 192 (Springer-Verlag Berlin Heidelberg, Berlin, Heidelberg, 2006).

I. Loshchilov and F. Hutter, CMA-ES for hyper-parameter optimization of Deep Neural Networks, arxiv:1604.07269 (2016).

M. Willjuice Ithurayaran and S. Baskar, Covariance matrix adaptation evolution strategy based design of centralized PID controller, Expert Systems with Applications 37, 5775 (2010).

I. Loshchilov, M. Schoenauer, and M. Sebag, Bi-population cma-es algorithms with surrogate models and line searches, in Proceedings of the 15th annual conference companion on Genetic and evolutionary computation (2013) pp. 1177–1184.

G. Kells, D. Meidan, and P. Brouwer, Near-zero-energy end states in topologically trivial spin-orbit coupled superconducting nanowires with a smooth confinement, Physical Review B 86, 100503 (2012).

E. Prada, P. San-Jose, and R. Aguado, Transport spectroscopy of n s nanowire junctions with majorana fermions, Physical Review B 86, 180503 (2012).

D. Rainis, L. Trifunovic, J. Klinovaja, and D. Loss, Towards a realistic transport modeling in a superconducting nanowire with Majorana fermions, Physical Review B 87, 024515 (2013).

J. Cayao, E. Prada, P. San-Jose, and R. Aguado, Sns junctions in nanowires with spin-orbit coupling: Role of confinement and helicity on the subgap spectrum, Physical Review B 91, 024514 (2015).

P. San-Jose, J. Cayao, E. Prada, and R. Aguado, Majorana bound states from exceptional points in non-topological superconductors, Scientific reports 6, 1 (2016).

J. Chen, P. Yu, J. Stenger, M. Hocevar, D. Car, S. R. Plissard, E. P. A. M. Bakkers, T. D. Stanescu, and S. M. Frolov, Experimental phase diagram of zero-bias conductance peaks in superconductor/semiconductor nanowire devices, Science advances 3, e1701476 (2017).

C.-X. Liu, J. D. Sau, T. D. Stanescu, and S. Das Sarma, Andreev bound states versus Majorana bound states in quantum dot-nanowire-superconductor hybrid structures: Trivial versus topological zero-bias conductance peaks, Physical Review B 96, 075161 (2017).

F. Peñaaranda, R. Aguado, P. San-Jose, and E. Prada, Quantifying wave-function overlap in inhomogeneous majorana nanowires, Physical Review B 98, 235406 (2018).

J. Avila, F. Peñaaranda, E. Prada, P. San-Jose, and R. Aguado, Non-hermitian topology as a unifying framework for the andreev versus majorana states controversy, Communications Physics 2, 1 (2019).

C.-K. Chiu and S. Das Sarma, Fractional Josephson effect with and without Majorana zero modes, Physical Review B 99, 035312 (2019).

J. Chen, B. D. Woods, P. Yu, M. Hocevar, D. Car, S. R. Plissard, Bakkers, E. P. A. M., T. D. Stanescu, and S. M. Frolov, Ubiquitous Non-Majorana Zero-Bias Conductance Peaks in Nanowire Devices, Physical review letters 123, 107703 (2019).

B. D. Woods, J. Chen, S. M. Frolov, and T. D. Stanescu, Zero-energy pinning of topologically trivial bound states in multiband semiconductor-superconductor nanowires, Physical Review B 100, 125407 (2019).

A. Vuik, B. Nijholt, A. Akhermov, and M. Wimmer, Reproducing topological properties with quasi-Majorana states, SciPost Physics 7, 061 (2019).

O. Dmytruk, D. Loss, and J. Klinovaja, Pinning of andreev bound states to zero energy in two-dimensional superconductor-semiconductor rashba heterostructures, Physical Review B 102, 245431 (2020).

E. Prada, P. San-Jose, M. W. de Moor, A. Geresdi, E. J. Lee, J. Klinovaja, D. Loss, J. Nygård, R. Aguado, and L. P. Kouwenhoven, From andreev to majorana bound states in hybrid superconductor–semiconductor nanowires, Nature Reviews Physics 2, 575 (2020).

M. Valentini, F. Peñaranda, A. Hofmann, M. Braunsch, R. Hauschild, P. Krogstrup, P. San-Jose, E. Prada, R. Aguado, and G. Katsaros, Nontopological zero-bias peaks in full-shell nanowires induced by flux-tunable andreev states, Science 373, 82 (2021).

H. Zhang, M. W. A. de Moor, J. D. S. Bommer, Di Xu, G. Wang, N. van Loo, C.-X. Liu, S. Gazibegovic, J. A. Logan, D. Car, Veld, Roy L. M. Op het, P. J. van Veldhoven, S. Koelling, M. A. Verheijen, M. Pendharkar, D. J. Pennachio, B. Shojaei, J. S. Lee, C. J. Palmstrom, E. P. A. M. Bakkers, S. D.arma, and L. P. Kouwenhoven, Large zero-bias peaks in InSb-Al hybrid semiconductor-
superconductor nanowire devices.

[79] L. Fu, Electron teleportation via Majorana bound states in a mesoscopic superconductor, Physical review letters 104, 056402 (2010).

[80] M. Hell, K. Flensberg, and M. Leijnse, Distinguishing Majorana bound states from localized Andreev bound states by interferometry, Physical Review B 97, 161401 (2018).

[81] A. M. Whiticar, A. Fornieri, E. C. T. O'Farrell, A. C. C. Drachmann, T. Wang, C. Thomas, S. Gronin, R. Kallasher, G. C. Gardner, M. J. Manfra, C. M. Marcus, and F. Nichele, Coherent transport through a Majorana island in an Aharonov-Bohm interferometer, Nature Communications 11, 3212 (2020).

[82] M. Thamm and B. Rosenow, Transmission amplitude through a Coulomb blockaded Majorana wire, Physical Review Research 3, 023221 (2021).

[83] C. Mahaux and H. A. Weidenmüller, Comparison between the R-matrix and eigenchannel methods, Physical Review 170, 847 (1968).

[84] C. W. Groth, M. Wimmer, A. R. Akhmerov, and X. Waintal, Kwant: a software package for quantum transport, New Journal of Physics 16, 063065 (2014).

[85] N. Hansen, Y. Akimoto, and P. Baudis, CMA-ES/pycma on Github, Zenodo, 10.5281/zenodo.2559634 (2019).

[86] See supplemental material.
A. AMPLITUDE OF COHERENT TRANSMISSION

As a metric for optimization, we use the amplitude of coherent transmission \(|T_{\uparrow\uparrow} + T_{\downarrow\downarrow}|\) through an Aharonov-Bohm interferometer, where \(T_{\sigma}\) is the quantum mechanical amplitude for an electron with spin \(\sigma\) to tunnel through the Majorana wire. The current through the interferometer is in leading order interference given by

\[
I = \frac{e^2}{h} \left\{ \sum_{\sigma \sigma'} |T_{\sigma \sigma'}|^2 + 2 |T_{\text{ref}}|^2 + I_{\text{inf}} \right\} \quad \text{(S1)}
\]

\[
I_{\text{inf}} = 2 \sum_{\sigma} \text{Re} \left[ e^{i \phi} T_{\sigma \sigma} T_{\text{ref}} \right] = \frac{e^2}{h} |T_{\text{ref}}|^2 \left[ e^{i \phi} (T_{\uparrow\uparrow} + T_{\downarrow\downarrow}) + e^{-i \phi} (T_{\uparrow\uparrow} + T_{\downarrow\downarrow})^* \right] \quad \text{(S2)}
\]

\[
= \frac{2e^2}{h} |T_{\text{ref}}|^2 |T_{\uparrow\uparrow} + T_{\downarrow\downarrow}| \cos(\phi + \gamma), \quad \text{(S3)}
\]

where \(T_{\uparrow\uparrow} + T_{\downarrow\downarrow} = |T_{\uparrow\uparrow} + T_{\downarrow\downarrow}| e^{i \gamma}\), the Aharonov-Bohm phase is denoted as \(\phi\), and the transmission through the reference arm \(T_{\text{ref}}\) is assumed to be real and diagonal in spin. Hence, the amplitude of interference oscillation is given by \(|T_{\uparrow\uparrow} + T_{\downarrow\downarrow}|\).

B. ALTERNATIVE METRICS AND THEIR SHORTCOMINGS

Here, we provide examples of optimizations of alternative metrics whose drawbacks are mentioned in the main text. First, we consider the direct conductance through the wire without an interferometer, which is easier to measure experimentally, but has the disadvantage of not being able to distinguish between ABSs and MZMs. This manifests itself in the optimization by yielding a pair of trivial near-zero energy levels (Fig. S1b), the ABSs, both of which are localized at the wire ends (Fig. S1a).

Another potential metric is the topological gap \(|\varepsilon_1 - \varepsilon_0|\), which, however, does not depend on the localization of the MZMs, nor does it rely on the presence of MZMs and the topological phase either. An optimization shows large \(|\varepsilon_1 - \varepsilon_0|\) (Fig. S2b), but the associated lowest level is not a Majorana state (Fig. S2a). In addition, \(\varepsilon_0 = 1.9 \cdot 10^{-8} E_{\text{so}}\) is also strongly reduced, which also shows that minimizing \(\varepsilon_0\) does not favor MZMs and can further be realized with ABSs.

Furthermore, we discussed problems related to suboptimal parameters. For the thermal average to reliably penalize ABSs, the temperature should be sufficiently high, and at the same time, of course, the temperature must be below the...
Figure S2. Results for gap optimization in a one dimensional wire in presence of disorder. We define the gap as the difference between the first two energy eigenvalues. We use 20 gates of equal size along the wire. (a) Wave function $|\Psi_0|^2$ of the the lowest level and corresponding hole and electron wave functions $|\nu_0|^2$ (orange) and $|\upsilon_0|^2$ (green). (b) Energies of the lowest ten Bogoliubov levels. (c) CMA-ES optimization result that maximizes the gap. (d) Disorder potential for $\sigma_{\text{dis}} = 50 E_{so}$ and $\lambda_{\text{dis}} = 0.052 l_w$. With the optimized gates, we observe an increased gap, however despite the lowest level being close to zero energy it is not a Majorana level as $|\upsilon_0| \neq |\upsilon_0|$. A critical temperature for preserving superconductivity. If one chooses too small temperatures, for example $T = 34$ mK, the optimization favors ABSs with energy slightly larger than temperature (Fig. S3) and also the gap above the ABS levels can be strongly reduced.

Figure S3. Results for transmission amplitude optimization in a one dimensional wire in presence of disorder but at very low temperature $\beta = 18 E_{so}^{-1}$. At very small temperatures an ABSs with low but finite energy has very different weight than a zero energy ABSs in the thermal average, such that the amplitude does not cancel when there are two ABSs with slightly split energy. We use 20 gates of equal size along the wire. (a) Wave function $|\Psi_i|^2$ of the the lowest level $i = 0$ (blue) and the second level $i = 1$ (red). (b) Energies of the lowest ten Bogoliubov levels. (c) CMA-ES optimization result that maximizes the gap. (d) Disorder potential for $\sigma_{\text{dis}} = 50 E_{so}$ and $\lambda_{\text{dis}} = 0.052 l_w$. With the optimized gates, we observe a diminished gap and a pair of ABSs near zero energy which are split by a small energy difference.

C. COMPUTATIONAL DETAILS

We use the pycma [2] python implementation of the CMA-ES [3, 4] algorithm, with an initial configuration $V_g(0) = 0$, the starting step size $\sigma(0) = 0.1 E_{so}$, population sizes of 80 or $4 + 3 \ln(N_g)$, and a seed of the pseudo random number generator of 12345678, if not specified otherwise. As algorithm termination conditions, we use topfun = $10^{-15}$, tolfunhist = $10^{-8}$, and tolx = $10^{-5}$ $E_{so}$. We note, however, that the potentials do not change significantly anymore much earlier to meeting these conditions, such that one can stop the optimization earlier in an experimental situation.

For the computation of the transmission amplitude, we use KWANT [1] to obtain several quantities. We define the lattice, onsite terms, and hopping terms using KWANT (Fig. S4) and extract the self energies $\Sigma_\alpha$ of lead $\alpha$, as well as the propagating modes $\phi_\alpha$ defined at the lead-wire interfaces. In addition, KWANT allows to extract the wire Hamiltonian $H_{\text{wire}}$, which we use to compute eigenstates $U_\nu$ and energy levels $\varepsilon_\nu$, from which we obtain the effective couplings and energy levels [5] used in the computation of the scattering matrix. For the Majorana wires, we consider an effective mass $m^* = 0.02 m_e$, Rashba spin orbit coupling strength $\alpha_{\text{R}} = 0.2$ eVÅ, a lattice spacing $a = 0.026 l_{so}$, and wire length $L = 13 l_{so}$. In addition, we set the chemical potential $\mu = 1 E_{so}$, the Zeeman energy $E_z = 6 E_{so}$, the proximity s-wave gap $\Delta = 2 E_{so}$, the charging energy $E_c = 8 E_{so}$, and the electron temperature $T = 183$ mK. In the wire, we use a steep confinement with $\sigma = 0.1 l_{so}$ and $V_0 = 65 E_{so}$ defined as $V_{\text{conf}}(y) = V_\sigma V_0 (y-x_0) + V_\sigma V_0 (y-L+x_0)$ such that the maxima are located close to the ends of the wire at $x_0$ and $L - x_0$ where $x_0$ is chosen such that the
Figure S4. Sketch of the Majorana wire model. We consider leads (red) and wire (blue) of length $L$ to be separated by a confinement potential $V_{\text{conf}}$ (green). Using the python package KWANT [1], we define the lattice Hamiltonian, extract the lead self energies $\Sigma_\alpha$, $\Gamma_\alpha$, propagating modes $\phi_\alpha$, and the wire Hamiltonian matrix $H_{\text{wire}}$ from which we obtain the eigenstates $U_w$ and energy levels $\varepsilon_w$.

The potential has decayed to $V_0/2$ at the ends of the wire.

Figure S5. Supercurrent distribution $j_S \propto \hbar m \nabla \theta + e m A$ at the left end of the two dimensional wire for the choice of vector potential $A$ and superconducting order parameter phase $\theta$.

The potential in the leads is given by $V_{\text{lead}} = -100 E_{so}$ to ensure that both spin components are present at the Fermi level. Leads are modeled with the Hamiltonian

$$H_{\text{lead}} = \tau_z \left[ -\frac{\hbar^2 \partial_y^2}{2m^*} \sigma_0 + V_{\text{lead}} \sigma_0 \right] - E_z \tau_0 \sigma_z .$$

(S4)

We consider gates of equal extension that start a distance $0.3 l_{so}$ from the ends of the wire to not interfere with the confinement potential which is produced by additional gates. Furthermore, we assume that the wire lies a distance $z_{\text{sys}} = 0.3 l_{so}$ above the gates (see main text Eq. (2)).

**D. TWO-DIMENSIONAL WIRE**

For the two dimensional case, we additionally choose a wire width $L_x = 0.39 l_{so}$, chemical potential $\mu = 63 E_{so}$, Zeeman energy $E_z = 6 E_{so}$, and otherwise the same parameters as in the one dimensional case. The full 2d Hamiltonian is given by

$$H_{\text{wire}}^{2d} = \tau_z \left[ -\frac{\hbar^2}{2m^*} (\partial_x^2 + \partial_y^2) \sigma_0 - \mu \sigma_0 - i\hbar \alpha_R (\sigma_x \partial_y - \sigma_y \partial_x) + \delta_{\text{dis}}(x,y) \sigma_0 + V_g(x,y) \sigma_0 + V_{\text{conf}}(y) \sigma_0 \right] + \frac{\mu g B_z}{2} \tau_0 \sigma_z + \Delta \tau_z \sigma_0 ,$$

(S5)

with Lande factor $g = -14.9$ [6], and we take into account the orbital effect of the magnetic field by adding a Peierls phase $e^{-ie/\hbar \int_A} A \cdot dr$ to the hoppings. We choose the phase of the superconducting order parameter as $\theta = 0$ and, away from the wire ends, the vector potential as $A = -B_z x \sigma_y$, so that it is independent of the coordinate $y$ along
the wire and the energy due to the supercurrent \( j_s = -2 e n_s (\hbar \nabla \theta + 2 e A)/m \) is minimized \([7]\). At the wire ends we use the following approximation to guarantee current conservation:

\[
A = -a(y) B_y x^y + \frac{a'(y)}{2} B_y (x^2 - (L_x/2)^2)x^y ,
\]

\[
a(y) = \begin{cases} 
  f_{y_L,y_L+\lambda}(y) & y_L \leq y > y_L + \lambda \\
  1 & y_L + \lambda \leq y \leq y_R - \lambda \\
  1 - f_{x_R-\lambda,x_R}(y) & y_R - \lambda < y \leq y_R 
\end{cases},
\]

\[
f_{y_1,y_2}(y) = \frac{h(y - y_1)}{h(y - y_1) + h(y_2 - y)}
\]

\[
h(y) = \begin{cases} 
  \exp(-\lambda/y) & y > 0 \\
  0 & y \leq 0 
\end{cases},
\]

which ensures that the vector potential at both ends \((x_L, x_R)\) of the wire vanishes over a distance \( \lambda = L_x/2 \) in a smooth manner. The resulting current \( j_s \) is shown in Fig. S5.

For computing the amplitude during optimization, we take into account the first ten effective energy levels, which speeds up the computations considerably, without influencing the transmission amplitude by a significant amount \([5]\). We verified this by evaluating the final transmission amplitude after optimization by taking into account 50 levels. In addition, we validated the amplitude in several cases at different steps during the optimization by considering all effective levels for single electron co-tunneling. We find that considering only ten levels during optimization adequately approximates taking the full number of levels into account, as it is relevant for an experiment.

![Figure S6](image)

**Figure S6.** Results for transmission through a two dimensional wire in the topological regime for optimization of the gates. We use 20 gates of equal size along the wire. Wave function \(|\Psi_0|^2\) of the lowest level for (a) the reference case without disorder and with zero gate voltage on all gates and (b) optimized gates without disorder (wave function engineering). (c) CMA-ES optimization result for the gate potential that maximizes the transmission amplitude. (d) Energies of the lowest five Bogoliubov levels for the reference case (red circles) and for the optimized gate potential (blue crosses).

**E. OPTIMIZATION IN THE SECOND SUBBAND OF THE TWO-DIMENSIONAL WIRE**

Gate optimization can also be fruitful for higher subbands, as we show in Fig. S7 where we consider the second topological phase for \( \mu = 144.5 \ E_{so}, \ E_z = 6 \ E_{so}, \ \Delta = 2 \ E_{so} \). However, in the presence of levels from different subbands near the Fermi level many subtleties arise that can distract the CMA-ES optimization, such that the optimization is not always able to restore MZMs in presence of disorder. Importantly, different subbands have very different coupling strengths to the leads, e.g. MZMs in the second subband might have smaller couplings than topologically trivial states from the first subband \([8]\). In order to mitigate this effect, we move both the superconductor and the first/last gate a distance \(1.04 L_{so}\) away from the ends of the wire, and add on-site disorder with strength \( \delta_{dis} = 100 \ E_{so} \) to the superconductor-free region \([8]\). Only moving the superconductor away from the ends and having gates in the normal-conducting regions at the ends would allow the effective chemical potential in the superconductor to change such that the optimization is less stable with the risk of moving completely out of the topological regime. Using
Figure S7. Results for transmission through a two dimensional wire in the topological regime in the second topological phase. Gates and superconductor are moved a distance $1.04 l_{so}$ away from the wire ends and onsite disorder with strength $100 E_{so}$ is added in the normal-conducting region to improve coupling of MZMs to the leads. We use 20 gates of equal size along the wire with $\mu = 244.5 E_{so}$, $E_z = 6 E_{so}$, and $\Delta = 2 E_{so}$. Wave function $|\Psi_0|^2$ of the lowest level for (a) the reference case without disorder and with zero gate voltage on all gates, (b) with bulk disorder ($\lambda_{dis} = 0.052 l_{so}$, $\delta_{dis} = 90 E_{so}$) before gate voltage optimization, and (c) with optimized gate voltages in the presence of disorder. (d) CMA-ES optimization result for the gate potential that maximizes the transmission amplitude. (e) Energies of the lowest five Bogoliubov levels for the reference case (red circles) and for the optimized gate potential (blue crosses).

In the modified setup, we find MZMs, which in the reference case without bulk disorder (Fig. S7a) couple about one order of magnitude stronger to the leads then other low energy levels. When adding bulk disorder (Fig. S7b), they are destroyed and low energy levels couple with similar strength to the leads, and after optimization (Fig. S7c), the MZMs are restored with a coupling about twice as strong as other low energy levels. Even with these modifications, in presence of higher subbands at the Fermi level, the occurrence of Andreev bound states and other strongly coupling non-topological low energy states cannot reliably be excluded making the optimization overall more fragile. On the other hand, this also shows that CMA-ES optimization helps with identifying weaknesses in a given setup, such that it can also be used as a tool to test ways to stabilize desired features in the system.

[1] C. W. Groth, M. Wimmer, A. R. Akhmerov, and X. Waintal, Kwant: a software package for quantum transport, New Journal of Physics 16, 063065 (2014).
[2] Nikolaus Hansen, yoshihikoueno, ARF1, Kento Nozawa, Matthew Chan, Youhei Akimoto, and Dimo Brockhoff, CMA-ES/pycma: r3.1.0 (Zenodo, 2021).
[3] N. Hansen and A. Ostermeier, Completely derandomized self-adaptation in evolution strategies, Evolutionary Computation 9, 159 (2001).
[4] N. Hansen, S. D. Müller, and P. Koumoutsakos, Reducing the time complexity of the derandomized evolution strategy with covariance matrix adaptation (CMA-ES), Evolutionary Computation 11, 1 (2003).
[5] M. Thamm and B. Rosenow, Transmission amplitude through a Coulomb blockaded Majorana wire, Physical Review Research 3, 023221 (2021).
[6] G. W. Winkler, A. E. Antipov, B. Van Heck, A. A. Soluyanov, L. I. Glazman, M. Wimmer, and R. M. Lutchyn, Unified numerical approach to topological semiconductor-superconductor heterostructures, Physical Review B 99, 245408 (2019).
[7] P. Wójcik and M. Nowak, Durability of the superconducting gap in majorana nanowires under orbital effects of a magnetic field, Physical Review B 97, 235445 (2018).
[8] F. Pientka, G. Kells, A. Romito, P. W. Brouwer, and F. Von Oppen, Enhanced zero-bias majorana peak in the differential tunneling conductance of disordered multisubband quantum-wire/superconductor junctions, Physical review letters 109, 227006 (2012).