Design and Optimization in Near-Term Quantum Computation

Aniruddha A. Bapat

Doctoral Defense

University of Maryland, College Park

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Overview of the thesis

- Near-term architectures
  - Ch. 2: When is an architecture “good” for quantum computation?
  - Ch. 3: Quantum protocols to move qubits over long distances
  - Ch. 4: Quantum routing: Qubit permutation algorithms
- Near-term algorithms

This talk

  - Ch. 5: Control of variational optimization algorithms
  - Ch. 6: Approximate state preparation on a trapped-ion quantum simulator
  - Ch. 7: Quantum-inspired optimization

List of publications (small = not in thesis)

- Ch. 2: Unitary entanglement construction in hierarchical networks. *Physical Review A*, *98*(6), 062328.
- Ch. 3: Nearly optimal time-independent reversal of a spin chain. *arXiv preprint arXiv:2003.02843*.
- Ch. 4: Quantum routing with fast reversals. *arXiv preprint arXiv:2103.03264.*
- Ch. 5: Bang-bang control as a design principle for classical and quantum optimization algorithms. *Quantum Info. Comput.* 19, 5–6 (May 2019), 424–446.
- Ch. 6: Quantum approximate optimization of the long-range Ising model with a trapped-ion quantum simulator. *Proceedings of the National Academy of Sciences*, *117*(41), 25396-25401.
- Ch. 7: Approximate optimization of the MaxCut problem with a local spin algorithm. *Physical Review A* 103, no. 5 (2021): 052413.
- Entanglement bounds on the performance of quantum computing architectures. *Physical review research*, *2*(3), 033316.
- Optimal protocols in quantum annealing and quantum approximate optimization algorithm problems. *Physical Review Letters*, *126*(7), 070505.
- Behavior of Analog Quantum Algorithms." *arXiv preprint arXiv:2107.01218* (2021).

Fall 2031, QIS 858: Scientific quantum computing

- Quantum simulation of QFT:
  - Representation, gauge symmetries
  - State preparation
  - Real-time dynamics

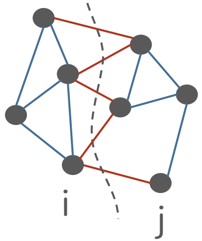
$$|\psi_{\text{free}}\rangle \xrightarrow{\text{QAO}} |\psi_{\text{interacting}}\rangle$$

Jordan, Lee, Preskill. *Science* 336.6085 (2012): 1130-1133.

- Quantum chemistry and material science:
  - *Ab initio* calculation of chemical energetics

$$H = \sum_{ij} A_{ij} a_i^\dagger a_j + \sum_{ijkl} B_{ijkl} a_i^\dagger a_j^\dagger a_k a_l$$

- Hard classical optimization:
  - Classical problems: Ising spin glasses, MaxCut, "QUBO", etc.



$$\longrightarrow \quad H = -\sum_{i<j} J_{ij} Z_i Z_j$$

NISQ = Noisy, Intermediate-Scale, Quantum

Preskill, *Quantum* 2 (2018): 79.
Egan, *et al.* & Brown, Monroe *arXiv:2009.11482* (2020).

Current capabilities are impressive, but limited. Over the next 5-10 years, quantum computers are likely to remain:

- Noisy: No fault tolerance. No/limited error-correction.
- Size-limited: 100-1000 qubits, low-depth circuits.
- Potentially non-universal: Limited set of feasible operations.
- Not fully connected: Restricted qubit connectivities such as chains, grids, modular hierarchies, etc.

... but when life gives you lemons, make lemonade!

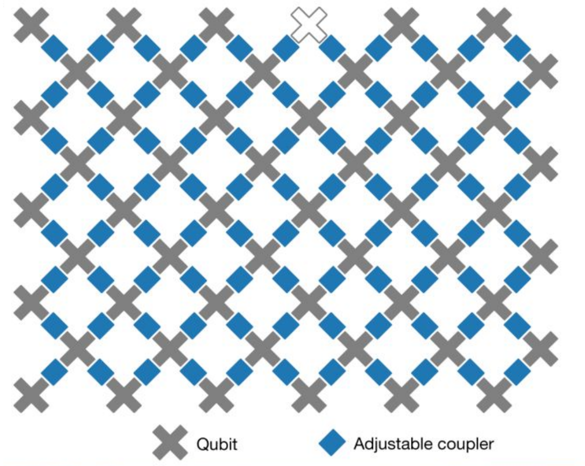
“Quantum lemonade”?

What can shallow-depth, noisy quantum circuits on ~100 qubits do?

Sample the output distribution of a random, low-depth circuit:

- Quantum computer on 53 qubits: 200 seconds
- Classical supercomputer: 10,000 years!

Aka “quantum supremacy”



Arute *et al* & Martinis (2019), Nature 574(7779) 505-510.

Takeaway: NISQ devices can prepare non-trivial quantum states that are beyond the scope of realistic classical computation.

Fall 2031, QIS 858: Scientific quantum computing

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Low-energy quantum state preparation

Quantum lemonade: Variational optimization

Goal: Find a state ψ that minimizes a figure of merit $E(\psi)$ approximately.

- ➤ $E(\psi) = \langle\psi|H|\psi\rangle$, H = Hamiltonian (classical cost, neg. ground state projector)
- ➤ But, n qubits ⇒ 2^n-dimensional Hilbert space. Bad news?

Strategy: Search over a smaller set of parameterized states,

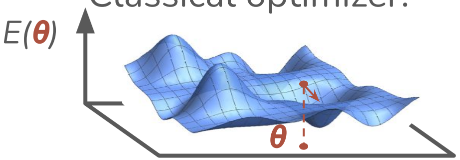
$|\psi(\boldsymbol{\theta})\rangle = U(\boldsymbol{\theta})\,|\psi_0\rangle$. Measure $E(\psi(\boldsymbol{\theta}))$ on a quantum computer.

Initial guess: $\boldsymbol{\theta}_0$ →

Quantum device: Prepare $\psi(\boldsymbol{\theta})$ and measure $E(\psi(\boldsymbol{\theta}))$

$E(\boldsymbol{\theta})$ ↑↓ $\boldsymbol{\theta}+\delta\boldsymbol{\theta}$

Classical optimizer:



→ Output: $\boldsymbol{\theta}^*$, $\psi(\boldsymbol{\theta}^*)$, E^*

Variational principle:

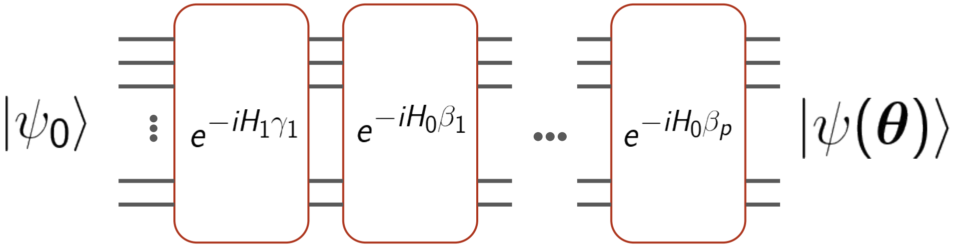
$\langle\psi|H|\psi\rangle \geq E_0$

Two prototypical variational algorithms

Quantum Approximate Optimization Algorithm (QAOA): Alternate between H_0, H_1 for p rounds.

Parameters: "Angles" $\{\beta_i\}_{i=1}^{p}$ and $\{\gamma_i\}_{i=1}^{p}$.

Target Hamiltonian: H_1 (e.g.)

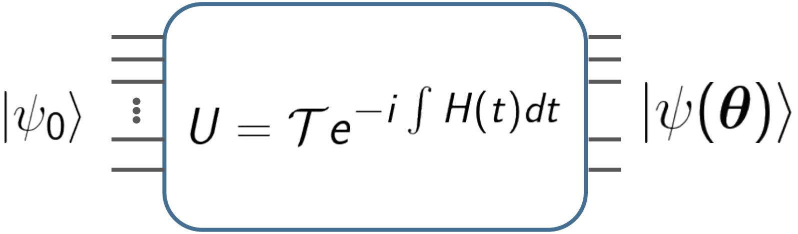


Farhi, Goldstone, Gutmann, *arXiv:1411.4028* (2014).

Peruzzo, Alberto, *et al. Nat. comm.* 5 (2014): 4213. (VQE)

Quantum Adiabatic Optimization (QAO): Evolve by *H(t)* slowly under smooth control *u(t)*.

$$H(t) = u(t)H_0 + (1 - u(t))H_1$$



Farhi, Goldstone, Gutmann, Sipser, *arXiv:quant-ph/0001106* (2000).

Kadowaki, T., & Nishimori, H. (1998). *Phys Rev E, 58*(5), 5355. (QA)

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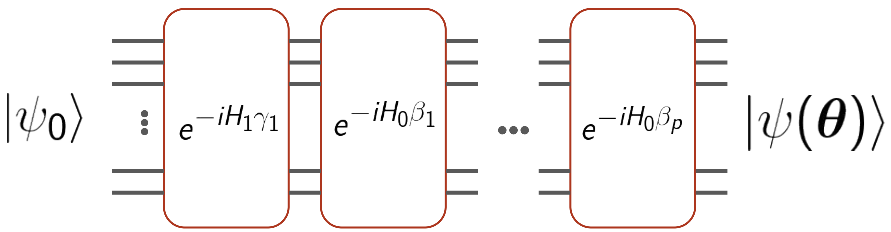
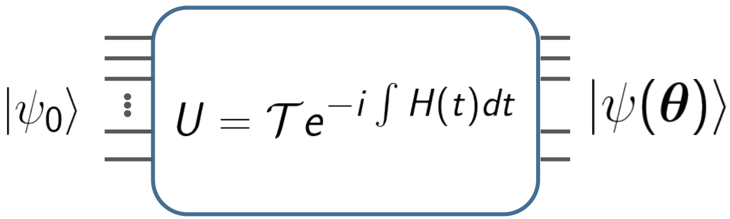
QAOA

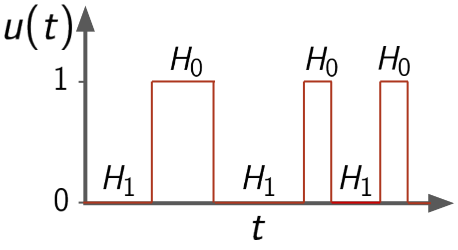


QAO

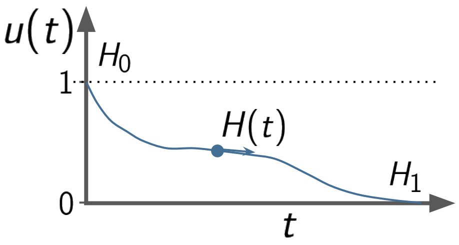


Evolve $\frac{d}{dt}|\psi\rangle = -iH(u(t))|\psi\rangle$, where $H(t) = u(t)H_0 + (1 - u(t))H_1$,

"Bang-bang" control



"Quasistatic" control



Goal: Design $u(t)$ such that at final time t_f, $E = \langle\psi(t_f)|H|\psi(t_f)\rangle$ is minimal.

How much does control matter?

AB and Stephen Jordan. *QIC* (2019).

Q: How large can the separation in performance between QAOA and QAO be?

Target Hamiltonian: Permutation-symmetric "ramp with a spike".

- **QAO:** Runtime dominated by smallest gap of H(t). Gap can be exponentially small.

  ⇒ Runtime ~ exp(n).

- **QAOA:** Prepares ground state with unit fidelity in 1 round.

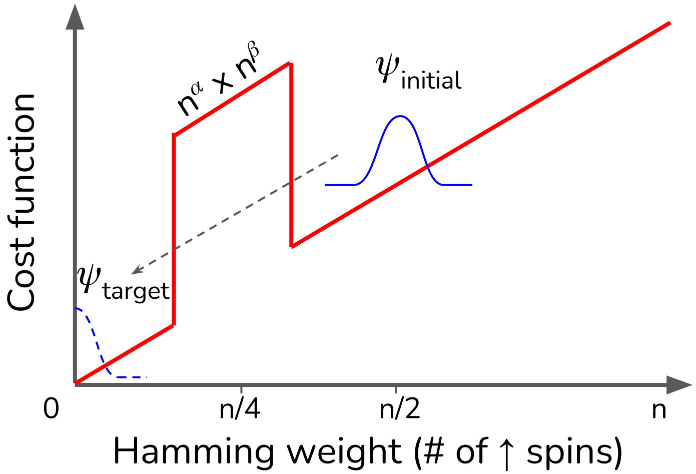
  ⇒ Runtime ~ O(1).

Ramp + Spike potential

$$r(w) = w$$

$$s(w) = \begin{cases} n^\beta, & \text{if } w \in [\frac{n}{4} - \frac{n^\alpha}{2}, \frac{n}{4} + \frac{n^\alpha}{2}] \\ 0, & \text{otherwise.} \end{cases}$$

$$c(w) = r(w) + s(w)$$



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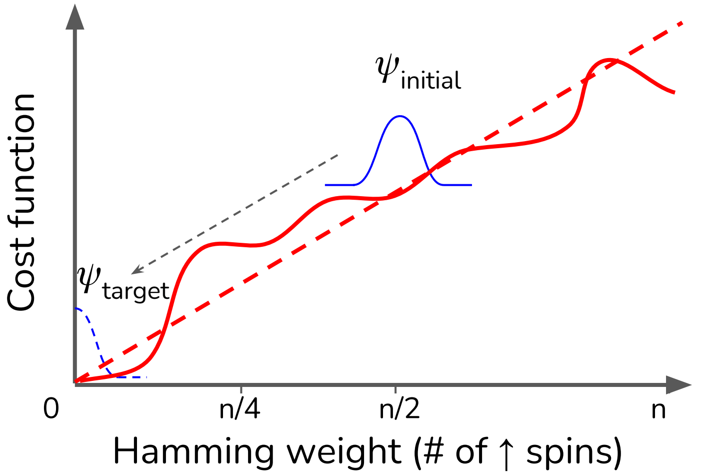
⇒ Runtime ~ O(1).

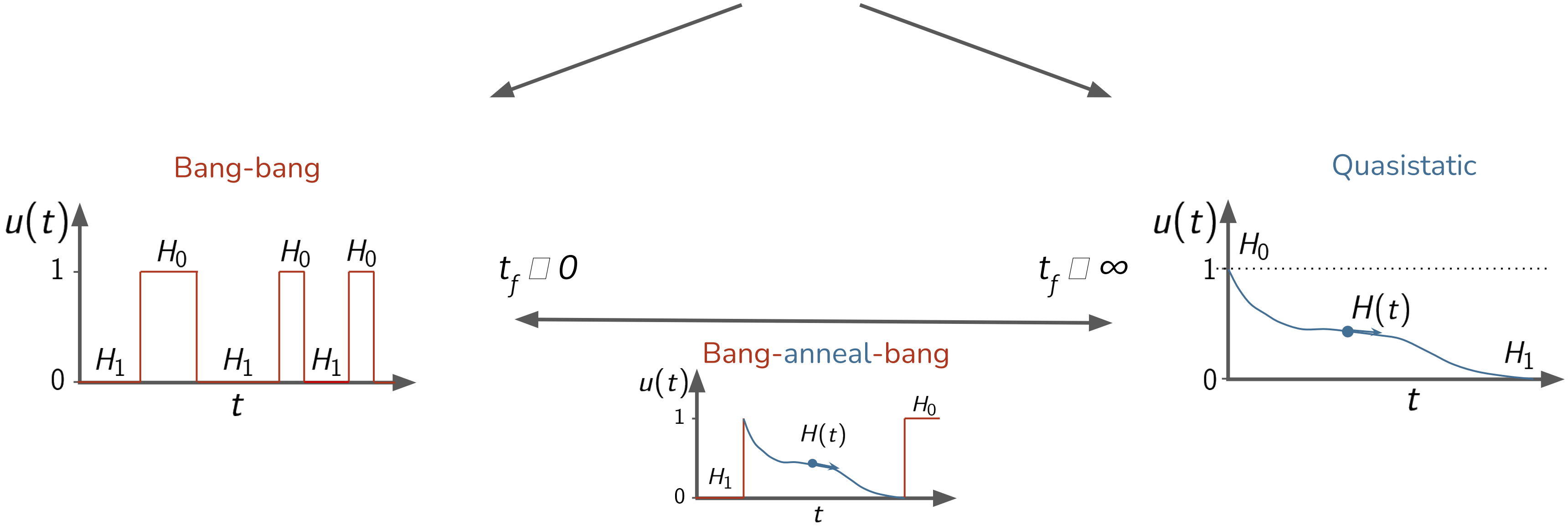
Locally ramp-like + "the rest" potential

$$c(w) = r(w) + s(w)$$



QAOA and QAO can be viewed as two limiting cases of a general, bang-anneal-bang control, where 'anneal' stands for an unspecified time dependence.

$$\frac{d}{dt}|\psi\rangle = -iH(u(t))|\psi\rangle \quad \text{where} \quad H(t) = u(t)H_0 + (1 - u(t))H_1$$



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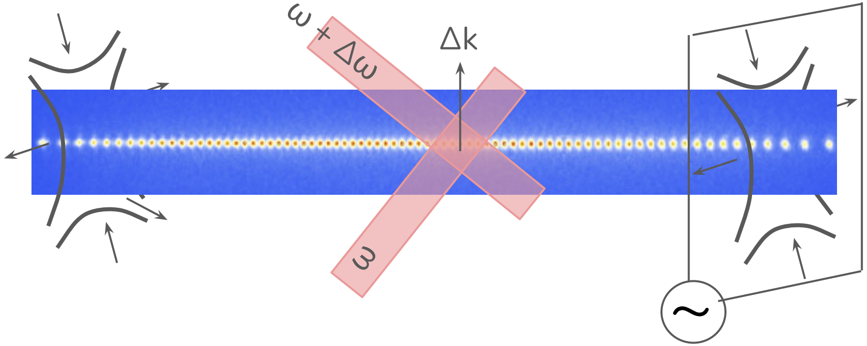
Experimental setup (Monroe Lab @ UMD)

Pagano, *et al.* *QST* 4.1 (2018): 014004.

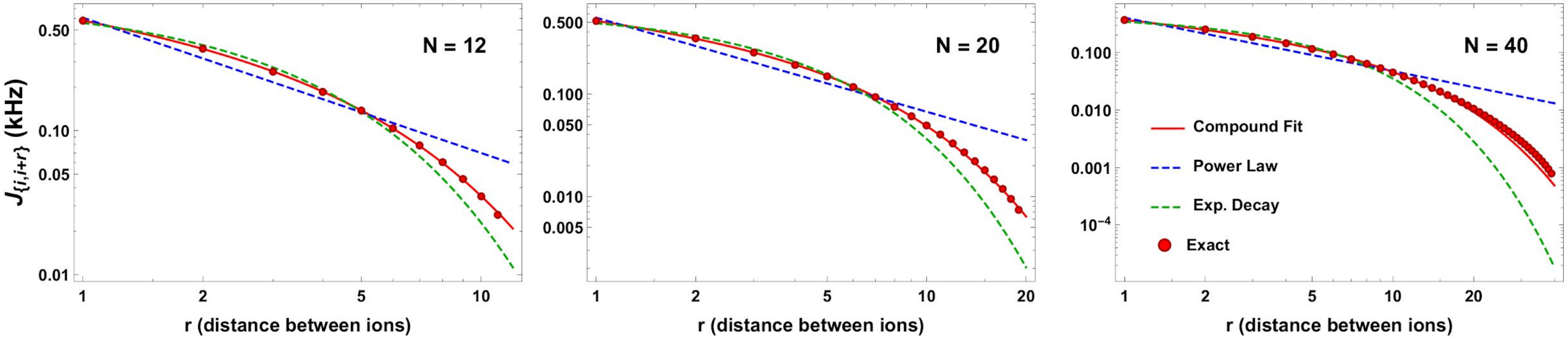
Kim, *et al.* *PRL* 103.12 (2009): 120502.

Linear Paul trap: Chain of $^{171}Yb^{+}$ ions confined (effectively) in all directions.



Global Pauli rotations + spin-dependent forces to generate two-body terms.

$$H = \sum_{i<j} J_{ij} Z_i Z_j - B \sum_i X_i$$

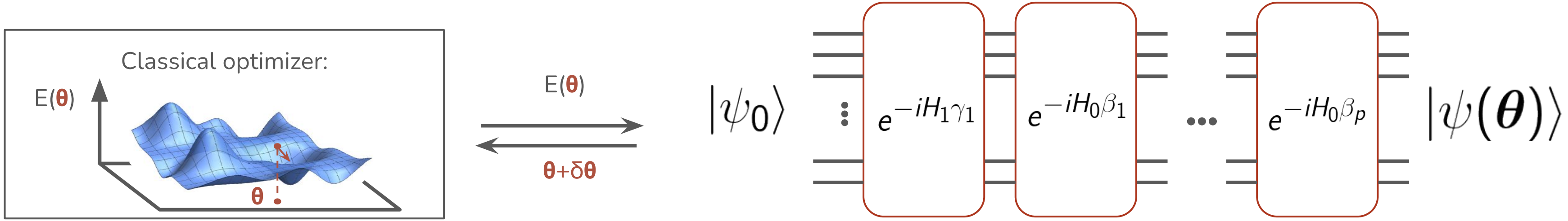


Ground state of the transverse-field Ising model

Pagano, **AB**, *et al.* (Jordan, Gorshkov, Monroe), *PNAS* 117.41 (2020): 25396-25401.

Goal: Approximate the ground state of

$$H = \underbrace{J_0 \sum_{i<j} \frac{1}{|i-j|^\alpha} Z_i Z_j}_{H_1} - B \underbrace{\sum_i X_i}_{H_0}$$



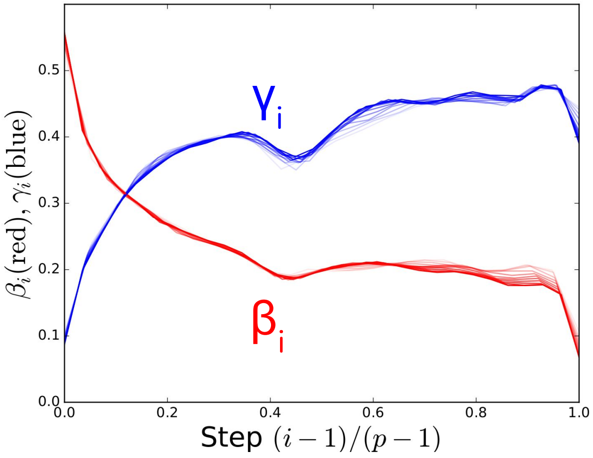
Budget: Ion chain has a finite lifetime, which limits number of calls to the quantum simulator. Brute-force optimization too expensive.

Observation: Optimal angles vary smoothly

Pagano, **AB**, *et al.* (Jordan, Gorshkov, Monroe), *PNAS* 117.41 (2020): 25396-25401.

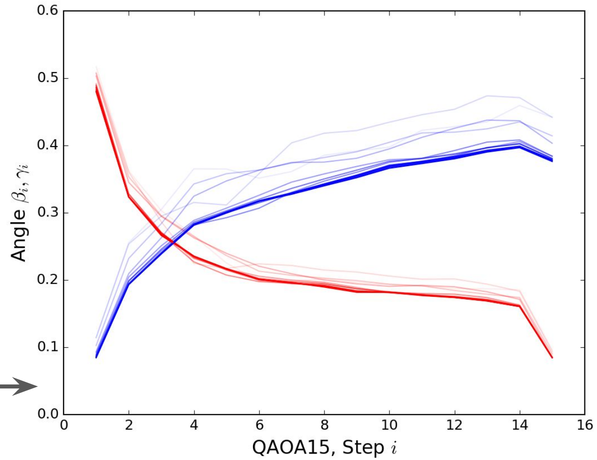
Optimal angles have structure: $\{\beta_i\}_{i=1}^{p}$ and $\{\gamma_i\}_{i=1}^{p}$ form smooth curves as a function of step i.

Moreover, *the curves converge for large N, large p (in fractional step number i/p)*.



← Left: N = 8, p = 20,21,...30

Right: p = 15, N = 8,9,...16 →

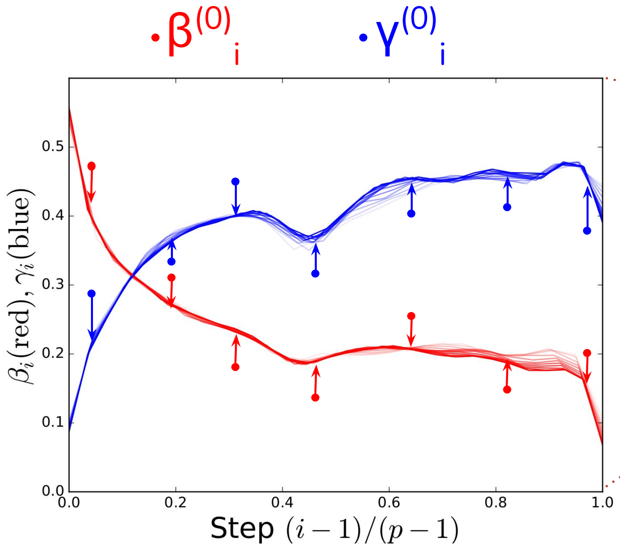


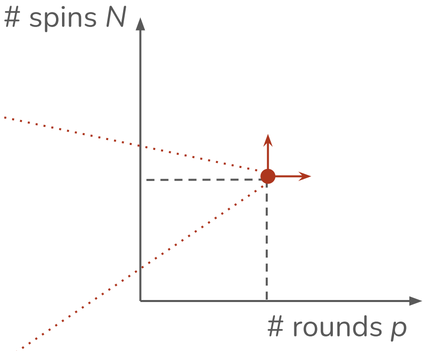
Clever guessing: Bootstrap heuristic

Pagano, **AB**, *et al.* (Jordan, Gorshkov, Monroe), *PNAS* 117.41 (2020): 25396-25401.

$\{\beta_i\}_{i=1}^{p}$ and $\{\gamma_i\}_{i=1}^{p}$ form a smooth curve as a function of step i (convergent in p,N).

- ➤ Start from small N,p.
- ➤ Learn the approximate curve.
- ➤ Extract an initial guess for larger N,p (via interpolation).





⇒ Brute force search not necessary!

Results

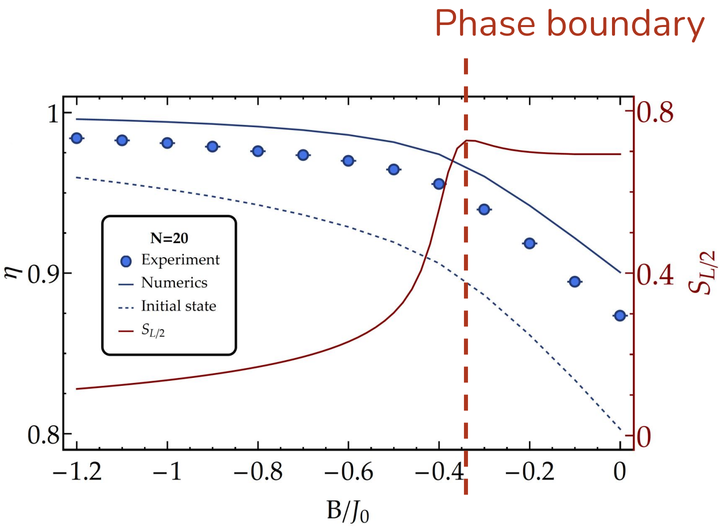
Pagano, **AB**, *et al.* & Jordan, Gorshkov, Monroe, *PNAS* 117.41 (2020): 25396-25401.

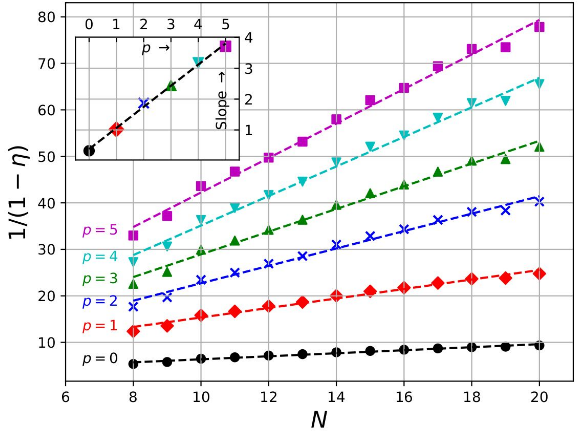
Brady, Kocia, Bienias, **AB**, Kharkov, & Gorshkov, A. V. (2021). *arXiv:2107.01218*.

- Good performance across phase diagram. Initial angle bootstrap heuristic + gradient descent (*p=1*,*2* and *N=12, 20, 40*.)

- Favorable scaling as p, N $\rightarrow \infty$. For a normalized energy η (1 = perfect), we find that $\eta \sim 1 - 1/(pN)$ for the critical ground state.

- Ongoing: The theory behind angle curves, their connection to annealing.





Outlook

- The NISQ era is a transitional stage in which physics experiments are “growing up” into quantum computers.
- It could be a while before we get fault-tolerant, universal quantum computers.
- NISQ devices can be powerful.
- Good design of algorithms and architectures will be the key to making the most of computation in this era (and to figure out how to get to the next era).
- Solutions designed to work in NISQ could also apply to the fault-tolerant era. (Example: parameterized circuits.)
- This is an exciting time to be doing quantum computation!

Thank you!

I thank my collaborators and friends at UMD:

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Chris Baldwin
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Abhinav Deshpande
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Lucas Kocia
Fangli Liu

Andrew Childs
Zohreh Davoudi
Zachary Eldredge
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Troy Sewell
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Niklas Mueller
Dhruv Devulapalli
Minh Tran
Andrew Guo

Arushi Bodas
Yidan Wang
Wen Lin Tan
Kaustubh Wagh
Jaideep Pathak
Sasha Mehan
Saikanth Dacha
Yogesh Balaji
Naren Manjunath
Subhayan Sahu
Papia Bera
(and so many more!)

Teaser: Routing

AB, Schoute, Gorshkov, Childs (2020), *arXiv:2003.02843*.
AB Shoute, King, Shastri, Gorshkov, Childs (2021), *arXiv:2103.03264*.

Qubit “routing” on incomplete graphs typically uses SWAP gates but these are:

- not always native to architecture,
- essentially classical.

Can we use “quantumness” of the data? Indeed!

- On the n-qubit chain, arbitrary permutations cost at most 2n/3 (vs. n),
- The addition of ancilla allows for $\sqrt{n}$ routing time (vs. n),
- Using measurement and fast classical feedback, a O(1) routing time (vs. log(n)).

Caveats to optimality of bang-bang

The optimality of bang-bang control has caveats:

1. Singular intervals: The optimal value of the control is determined by switching function Φ(t),

$$\Phi(t) = d\mathcal{H}/dt, \quad u^*(t) = \begin{cases} 1, & \text{if } \Phi(t) < 0, \\ 0, & \text{if } \Phi(t) > 0. \end{cases}$$

   When Φ(t) = 0 over a “singular” time interval, the optimal form may not be bang-bang there.

2. Infinite switches (aka *Fuller phenomenon*), etc.

AB and Stephen Jordan. *QIC* 19.5-6 (2019): 424-446.

Runtimes

Instance	Annealing-based		Bang-bang	
	QAO	SA	QAOA	BBSA
Bush, $\lambda \geq 1$	poly(n) [13]	exp(n) [13]	$O(1)$§ 8.3.2	$\tilde{O}\left(n^{3.5\cdots}\right)$§ 8.2.1
Bush, $\lambda < 1$	exp(n) [13]	exp(n) [13]	$O(1)$§ 8.3.2	$\tilde{O}\left(n^{3.5\cdots}\right)$§ 8.2.1
Spike, $2\alpha + \beta \leq 1$	poly(n) [14]	exp(n) [13]	$O(1)$§ 8.3.1	$O(n)$§ 8.2.2
Spike, $2\alpha + \beta > 1$	exp(n) [14]	exp(n) [13]	$O(1)$§ 8.3.1	$O(n)$§ 8.2.2

The heuristic optimization alignment chart

QUASISTATIC ⟷ BANG-BANG

QUANTUM ⟷ CLASSICAL

QUANTUM / QUASISTATIC: Quantum Adiabatic Optimization (QAO)

$$H_0 = -\sum_{i=1}^{n} X_i \qquad H_1 = \sum_{z\in\{0,1\}^n} c(z)|z\rangle\langle z|$$

$$|\psi(u=0)\rangle \xrightarrow{\text{quasistatic}} |\psi(u=1)\rangle$$

QUANTUM / BANG-BANG: Quantum Approximate Optimization Algorithm (QAOA)

$$H_0 = -\sum_{i=1}^{n} X_i \qquad H_1 = \sum_{z\in\{0,1\}^n} c(z)|z\rangle\langle z|$$

$$|+\rangle^{\otimes n} \equiv |\psi_0\rangle \xrightarrow{e^{-i\gamma_1 H_1}} |\psi_1\rangle \xrightarrow{e^{-i\beta_1 H_0}} \cdots \xrightarrow{e^{-i\beta_p H_0}} |\psi_{2p}\rangle$$

$$E(\vec{\beta},\vec{\gamma}) = \langle \vec{\beta},\vec{\gamma}|H_1|\vec{\beta},\vec{\gamma}\rangle$$

CLASSICAL / QUASISTATIC: Simulated Annealing (SA)

Metropolis-Hastings Monte Carlo with temperature schedule:

$$\infty \longrightarrow \cdots \longrightarrow T \longrightarrow \cdots \longrightarrow 0$$

and flipping probability:

$$1 \longrightarrow \cdots \min\left\{1, e^{-\Delta_{\text{flip}}V/T}\right\} \cdots \longrightarrow \Theta(\Delta_{\text{flip}}V)$$

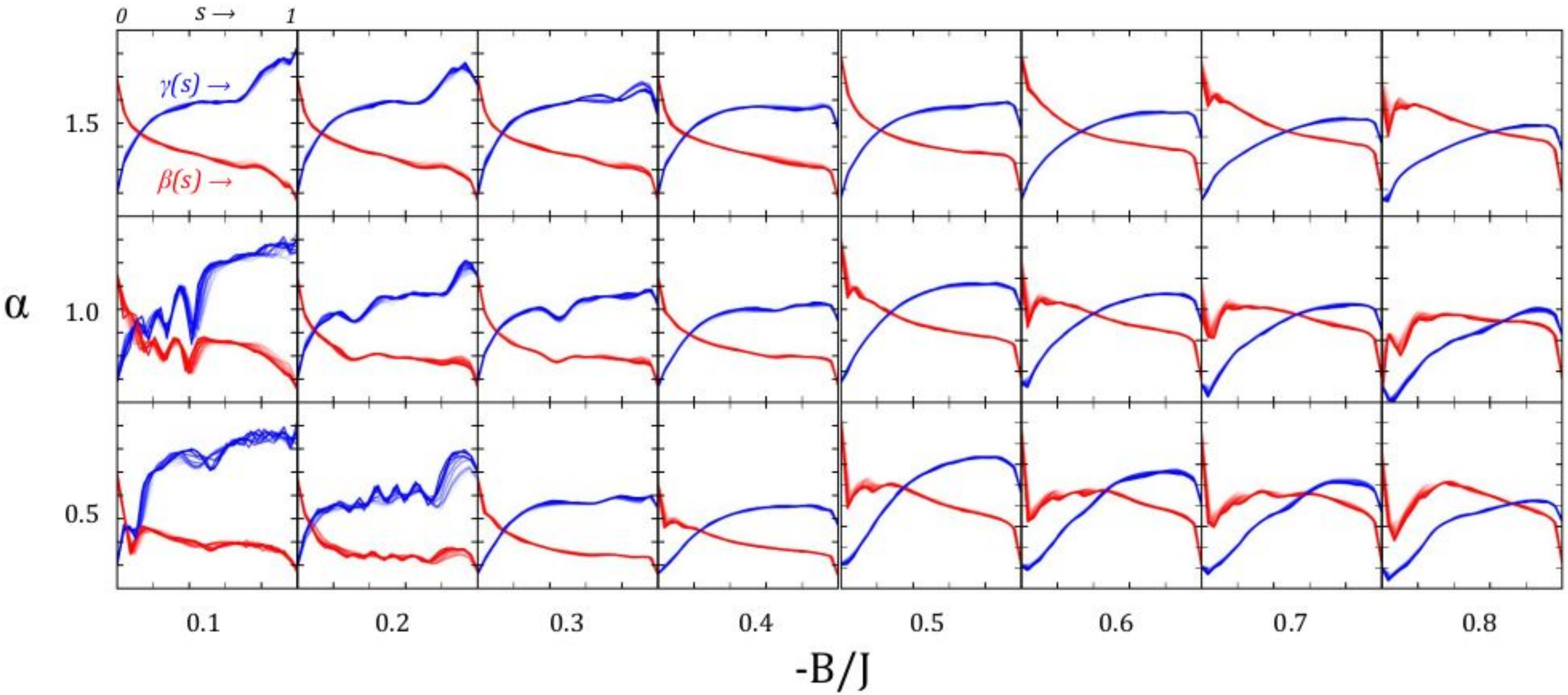
Diffusion … Randomized descent

CLASSICAL / BANG-BANG: Bang-bang Simulated Annealing (BBSA)

We run MH Monte-Carlo with a bang-bang schedule, i.e., only allowing T = 0,∞ .

This corresponds to alternating periods of randomized descent and diffusion.

Optimal curves across the phase diagram



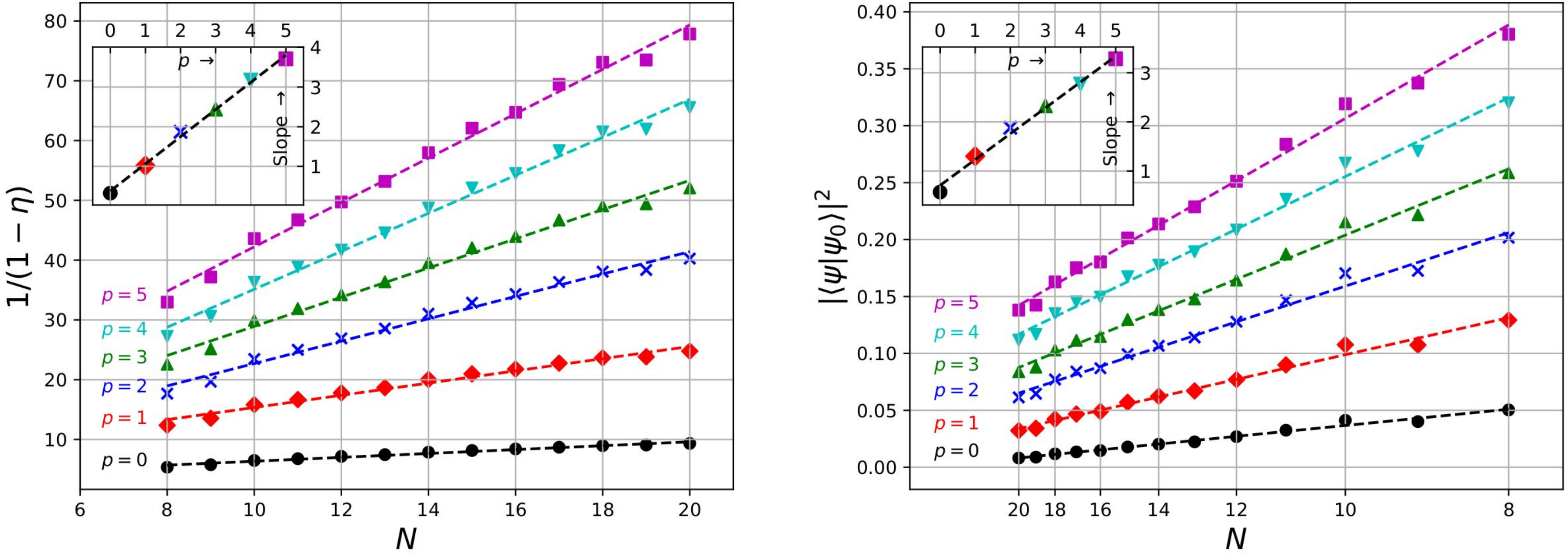
Pagano, G, **AB,** et al. *PNAS* 117.41 (2020): 25396-25401.

Performance scaling

η: Normalized energy (1 = ground state, 0 = highest excited state).

$|\langle\psi|\psi_0\rangle|^2$: Ground state probability.

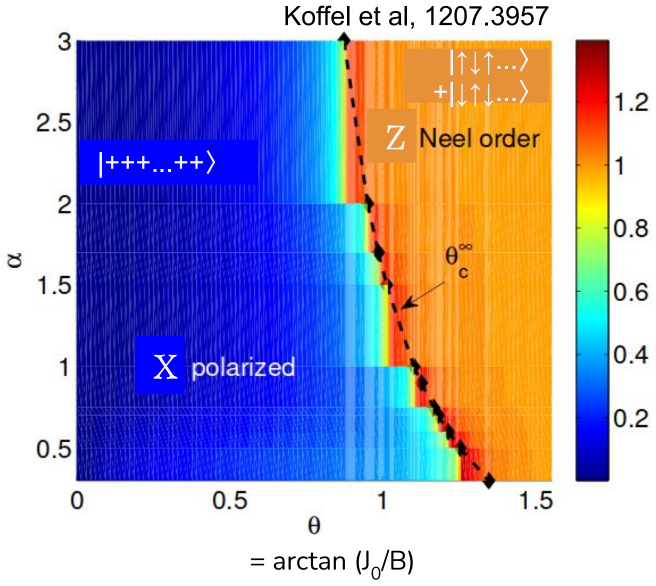
From numerics, $\eta \sim 1 - 1/(pN)$, $|\langle\psi|\psi_0\rangle|^2 \sim p/N$

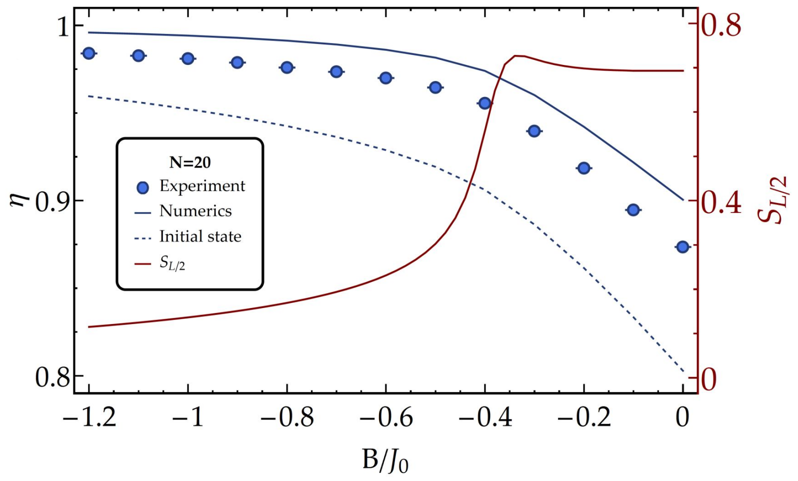


Pagano, G, **AB,** et al. *PNAS* 117.41 (2020): 25396-25401.

QAOA across the phase transition

The phase diagram two-dimensional, with parameters α and arctan(J_0/B). There are two phases, Z-aligned and X-aligned as shown. QAOA performs well at criticality. Performance is smooth across the boundary.

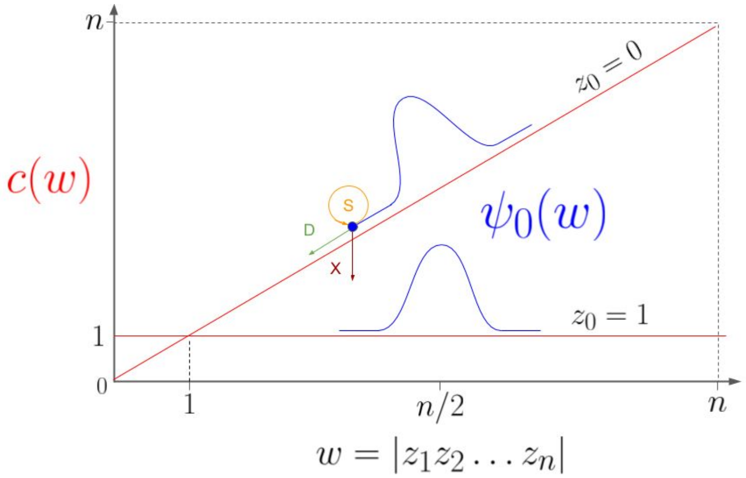




Both toy models

Hamming symmetry: c(z) ≡ c(w), where w = |z| = # of ones in the bit string z

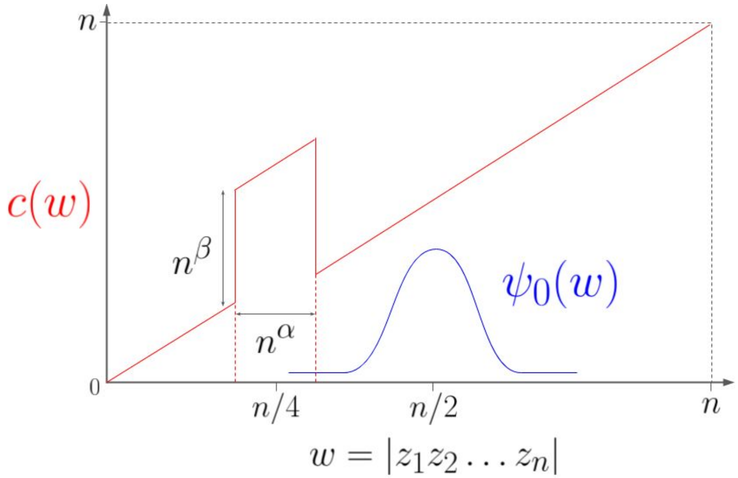
1. Bush of Implications (Bush)



$$c(z_0 z_1 \dots z_n) = z_0 + \sum_{i=1}^{n} z_i(1 - z_0)$$

$$c(z_0, w) = z_0 + w(1 - z_0)$$

2. Ramp with Spike (Spike)



$$r(w) = w, \quad s(w) = \begin{cases} n^\beta, & \text{if } w \in [\frac{n}{4} - \frac{n^\alpha}{2}, \frac{n}{4} + \frac{n^\alpha}{2}] \\ 0, & \text{otherwise.} \end{cases}$$

$$c(w) = r(w) + s(w)$$