USC Viterbi School of Engineering

ISI Information Sciences Institute

Adiabatic quantum machine learning

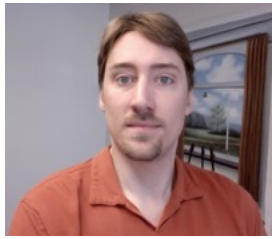
Sergio Boixo
Information Sciences Institute
USC Viterbi School of Engineering
Harvard Associate

USC Viterbi School of Engineering

People at USC / ISI

ISI Information Sciences Institute

Federico Spedalieri



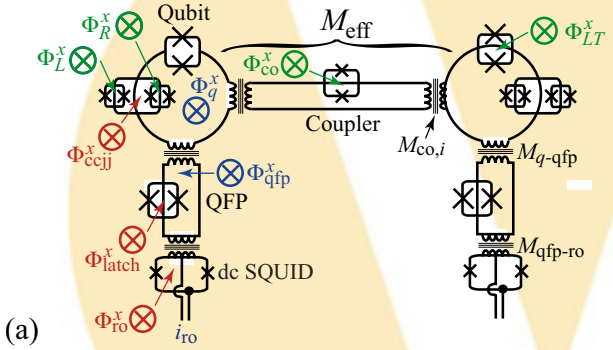
Greg Ver Steeg

Kristen Pudenz

Daniel Lidar

Stephan Haas
Paolo Zanardi
Todd Brun
Lorenzo Campos
Tony Levi
Edmun Jonckheere
Massoud Pedram
Susumu Takahashi

Bob Lucas
John Damoulakis



(a)

USC Viterbi School of Engineering

Adiabatic quantum machine learning

ISI Information Sciences Institute

- H. Neven, V. S. Denchev, M. Drew-Brook, J. Zhang, W. G. Macready, and G. Rose, "NIPS 2009 Demonstration: Binary Classification using Hardware Implementation of Quantum Annealing," 2009.
- H. Neven, V. S. Denchev, G. Rose, and W. G. Macready, "Training a Binary Classifier with the Quantum Adiabatic Algorithm," 0811.0416, Nov. 2008.
- H. Neven, V. S. Denchev, G. Rose, and W. G. Macready, "Training a Large Scale Classifier with the Quantum Adiabatic Algorithm," 0912.0779, Dec. 2009.
- H. Neven, G. Rose, and W. G. Macready, "Image recognition with an adiabatic quantum computer I. Mapping to quadratic unconstrained binary optimization," 0804.4457, Apr. 2008.
- K. L. Pudenz and D. A. Lidar, "Quantum adiabatic machine learning," 1109.0325, Sep. 2011.

USC Viterbi School of Engineering

Aspuru-Guzik group

ISI Information Sciences Institute

USC Viterbi School of Engineering

Clean Energy Project

ISI Information Sciences Institute

@ Harvard:

Prof Alán Aspuru-Guzik
Dr Johannes Hachmann
Dr Şule Atahan-Evrenk
MSc Roberto Olivares-Amaya
Prof Carlos Amador-Bedolla (UNAM, Mexico)
former: Dr Roel S. Sánchez-Carrera (now Bosch)
MSc Leslie Vogt
Aryeh Gold-Parker
Anna Brockway (REU)
Aidan Daly

@ Stanford:

Prof Zhenan Bao
Dr Rajib Mondal
Dr. Tony Sokolow

@ Q-Chem Inc.:

Dr Yihan Shao
Dr Alex Sodt
Dr Zhenting Gan
Dr Jing Kong

@ IBM WCG:

Bill Bovermann
Jonathan Armstrong
Kevin Reed
Keith Uplinger

@ USC - ISI:

Sergio Boixo

USC Viterbi School of Engineering

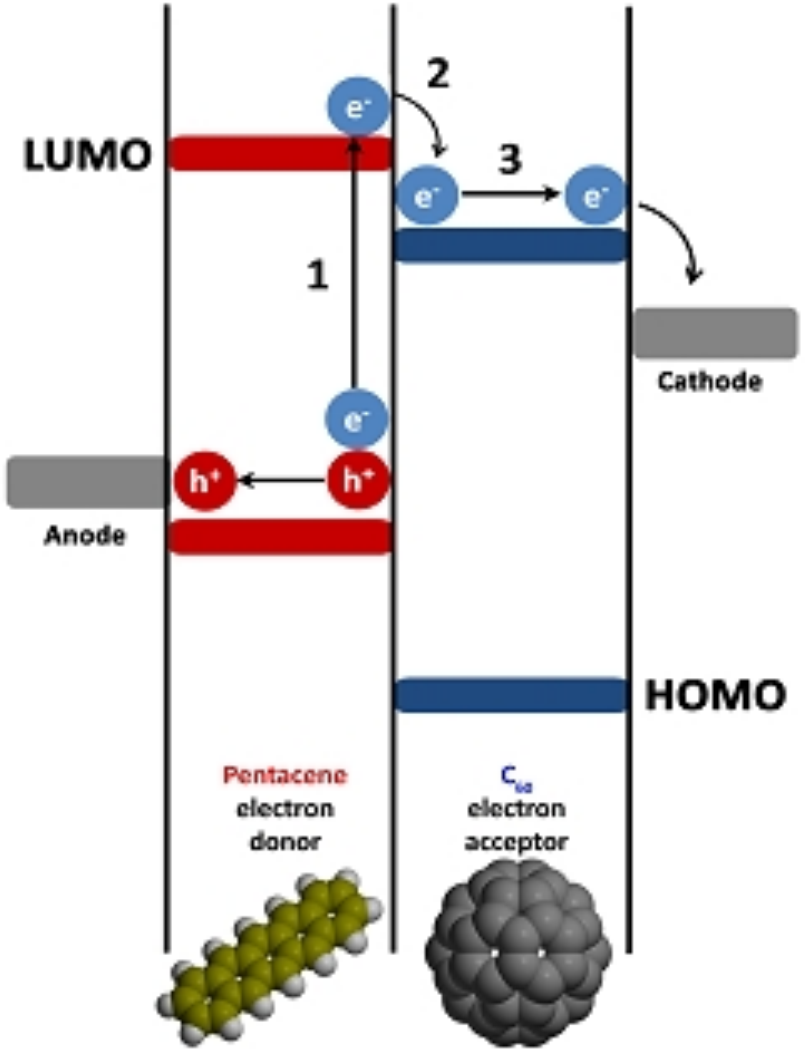
Clean Energy Project

ISI Information Sciences Institute

USC Viterbi School of Engineering

Organic photovoltaics 101

ISI Information Sciences Institute

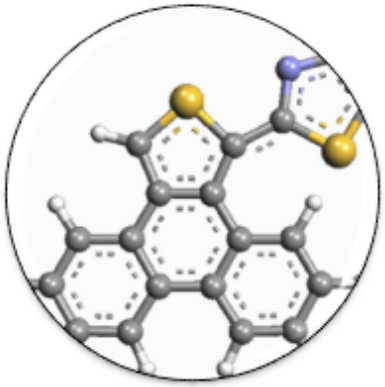


- Exciton formation
- Exciton diffusion
- Charge separation
- Charge transport
- Injection onto electrodes

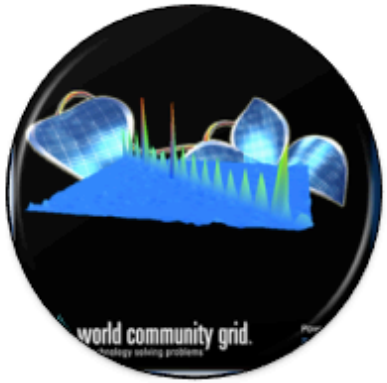
USC Viterbi School of Engineering

CEP Steps

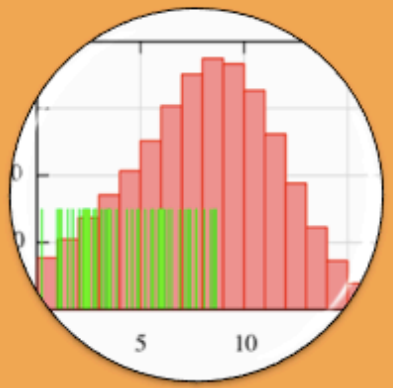
Information Sciences Institute



Molecule Generation



Quantum chemistry by distributed computing

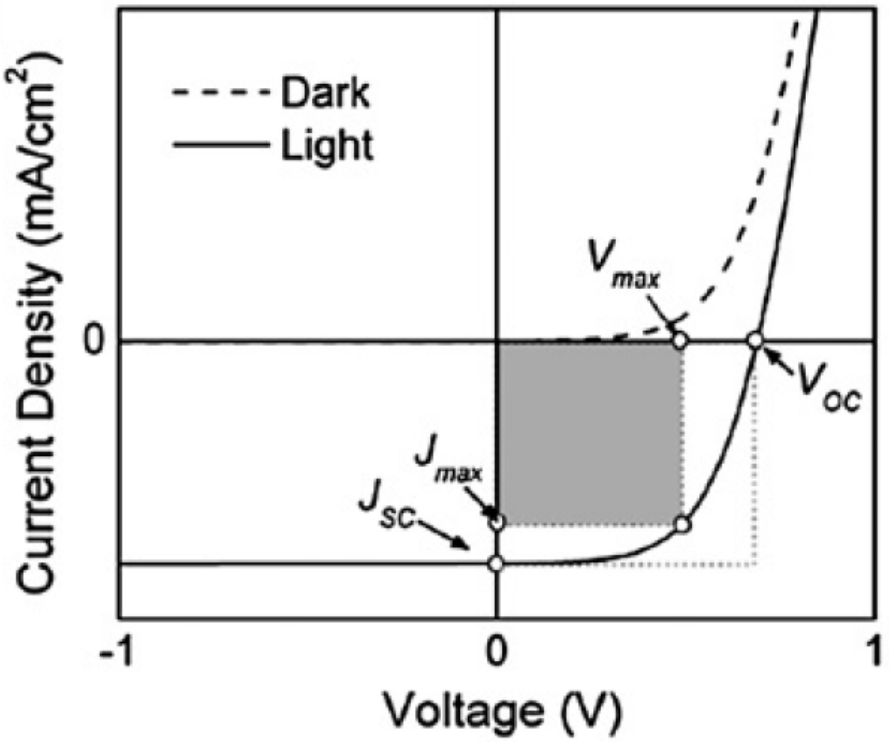


Cheminformatics

USC Viterbi School of Engineering

%Power Conv. Effic.

ISI Information Sciences Institute



Jsc – Short-circuit current

Voc – Open-circuit voltage

FF – Fill factor

$$\%PCE = \frac{J_m V_m}{P_{in}} = FF\frac{J_{sc}V_{oc}}{P_{in}}$$

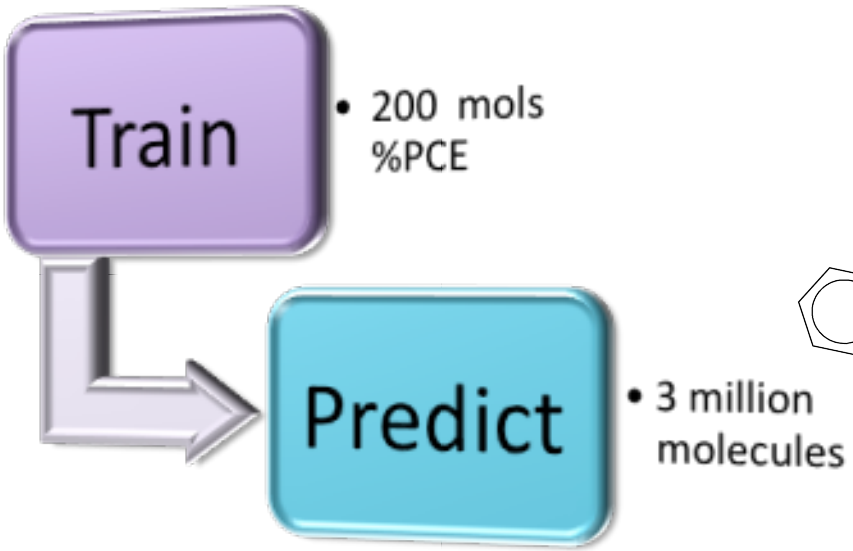
For different families:
3.3% -> 7.7%

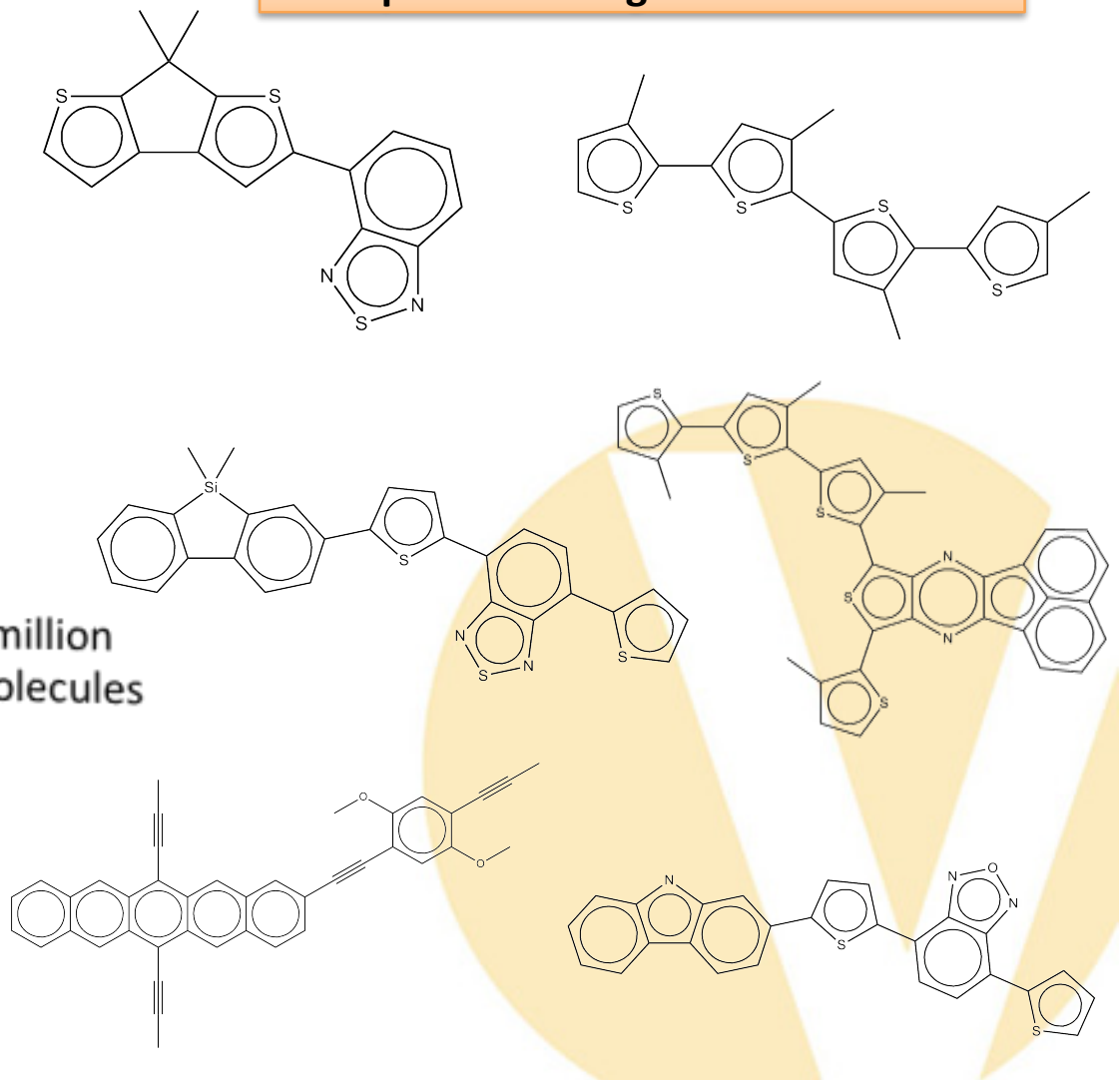
USC Viterbi School of Engineering

CEP Machine Learning

Information Sciences Institute

Example of training set molecules

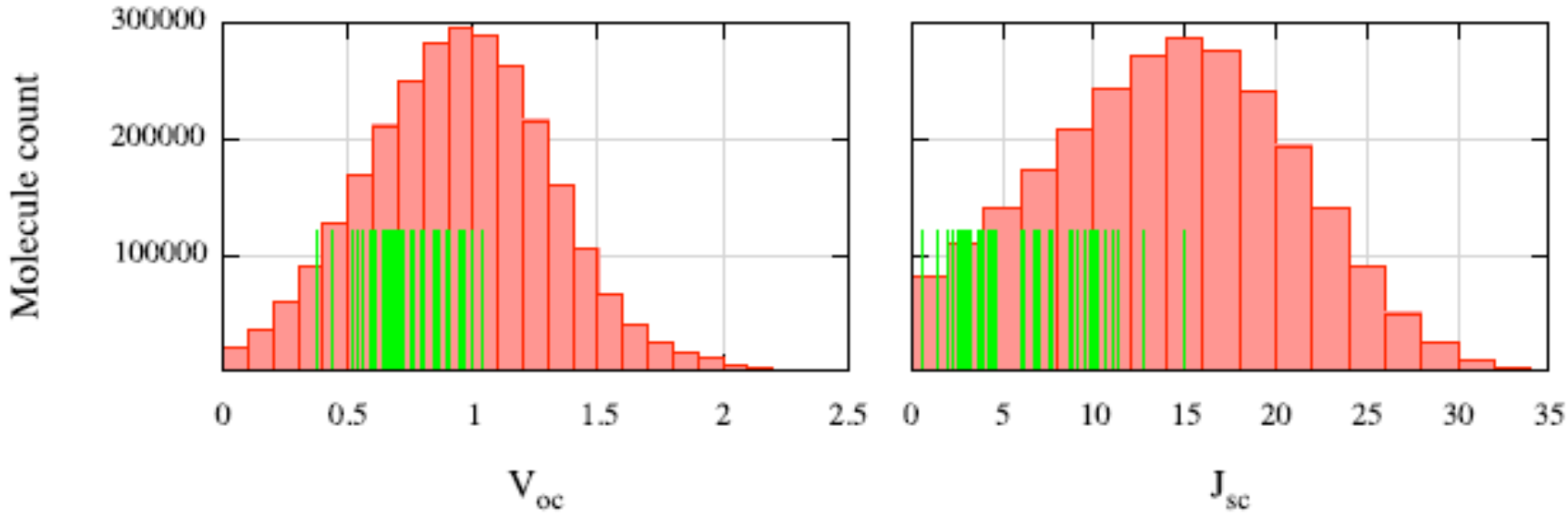




USC Viterbi School of Engineering

Results with lin. reg.

ISI Information Sciences Institute

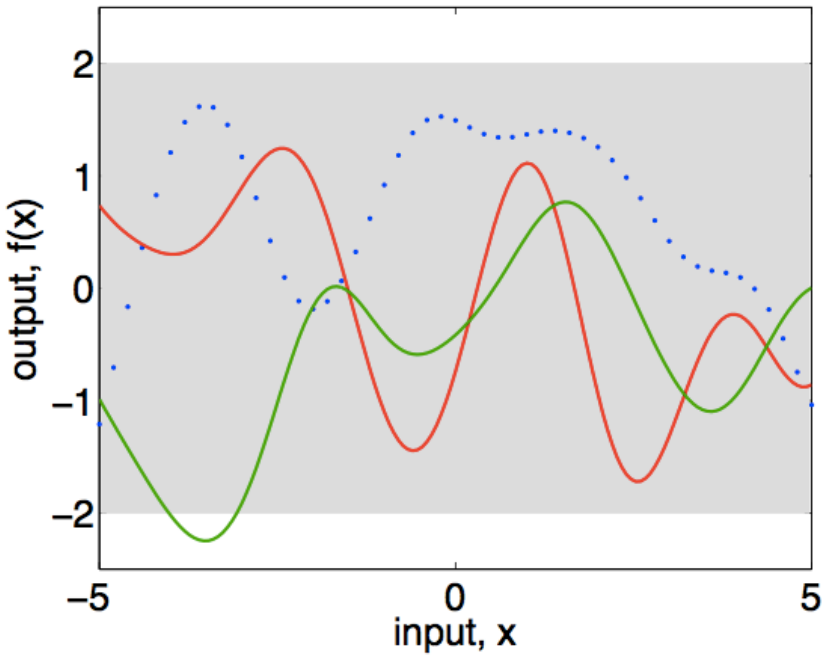


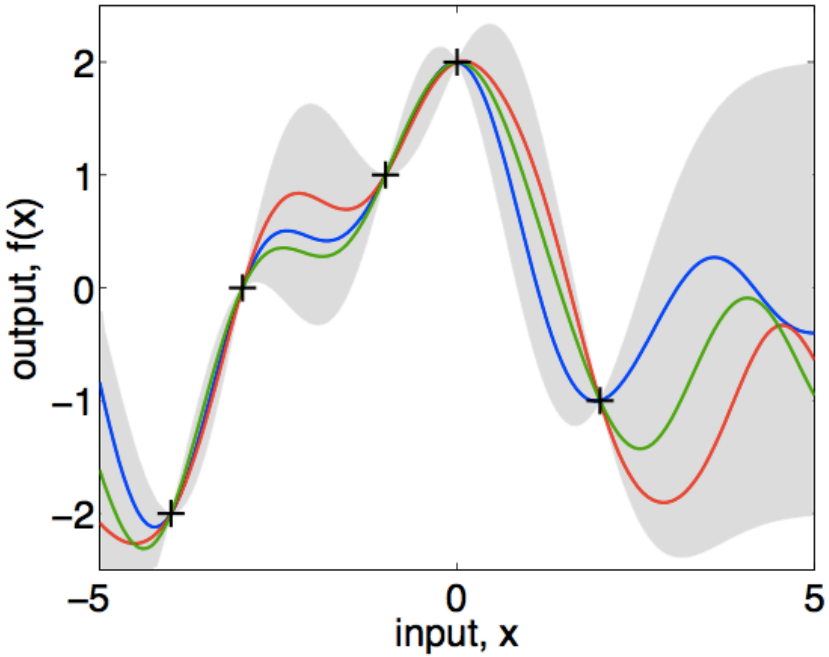
Olivares-Amaya, Amador-Bedolla, Hachmann, Atahan-Evrenk, *et al.*. *Energy Environ. Sci.* (2011)

USC Viterbi School of Engineering

Gaussian Processes

ISI Information Sciences Institute



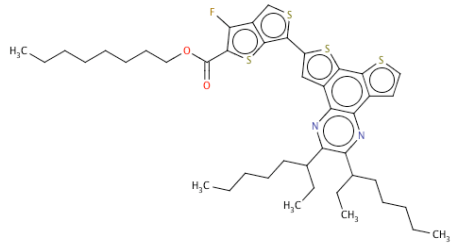


- High-level Gaussian distribution over functions
- Gray area defines where the function could be - defined entirely by mean and standard deviation
- As you add data points, you become more certain of the behavior of the function near those points

USC Viterbi School of Engineering

Binary Classification
Feature Selection

ISI Information Sciences Institute



Dragon 6

MW	Amw	Me	Mp	Mi	nBP	…
0	0	1	0	1	0	…

< 0 0 1 0 1 0 … >

✔

PCE ≥ 6.5

- Rather than predicting numerical value for efficiency, predicts whether or not it will be over a certain threshold
- Solution is a binary vector marking each descriptor as a "good predictor" or "bad predictor"
- Reduces descriptor space at expense of complexity of output

USC Viterbi School of Engineering

Burden Matrix

Structural information

ISI Information Sciences Institute

Symmetric matrix of atomic entries with:

- Atomic number in the diagonal
- Off-diagonal:
  - Conventional bond order / 10. (Conventional bond order is 0.1, 0.2, 0.3 and 0.15 for single, double, triple and aromatic bonds).
  - Terminal bonds: + 0.01
  - Other entries: +0.001

Typical descriptor: SpMax_Bh(m), second largest eigenvalue.

USC Viterbi School of Engineering

Moran Autocorrelation

ISI Information Sciences Institute

$$\frac{\frac{1}{\Delta_k} \cdot \sum_i \sum_j (w_i - \bar{w}) \cdot (w_j - \bar{w}) \cdot \delta(d_{ij}, k)}{\frac{1}{A} \cdot \sum_i (w_i - \bar{w})^2}$$

Typical descriptor: MATS5m, Moran autocorrelation of lag 5 weighted by mass.

USC Viterbi School of Engineering

Machine learning "Boosting"

ISI Information Sciences Institute

We start with "weak classifiers" that are correct with some probability:

$$h_j(x) = \begin{cases} 1 & \text{if } x \textit{ seems} \text{ of type } 1 \\ 0 & \text{if } x \textit{ seems} \text{ of type } 0 \end{cases}$$

One classifier for each descriptor

We find a strong classifier:

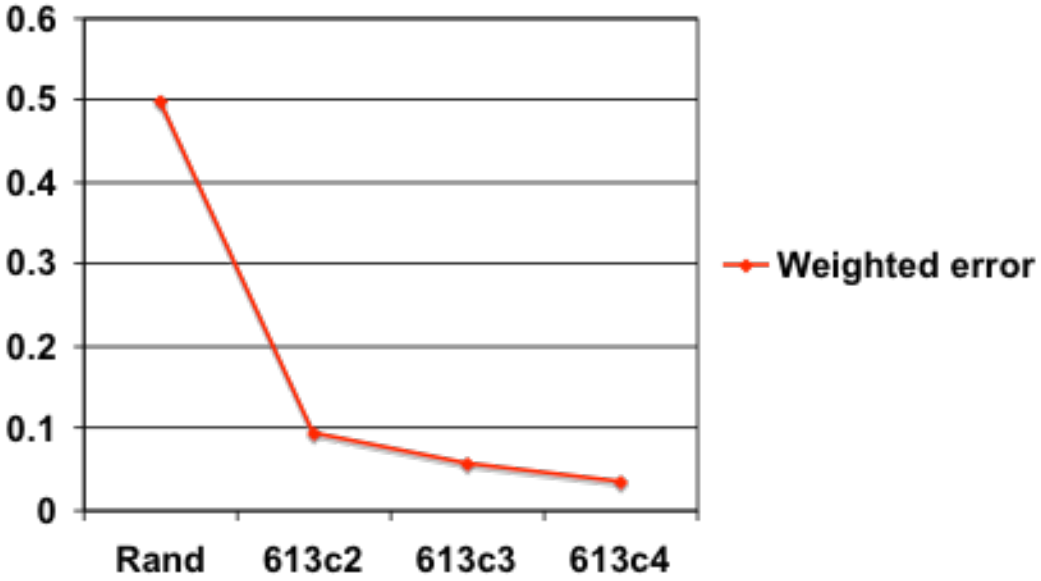
$$H(x) = \left(\sum_j \omega_j h_j(x) > T \right)$$

H. Neven, V. S. Denchev, G. Rose, W. G. Macready 2008, 2008, 2009, 2009. K. Pudenz, D. Lidar 2011

USC Viterbi School of Engineering

Exhaustive Search for Strong Classifier

ISI Information Sciences Institute

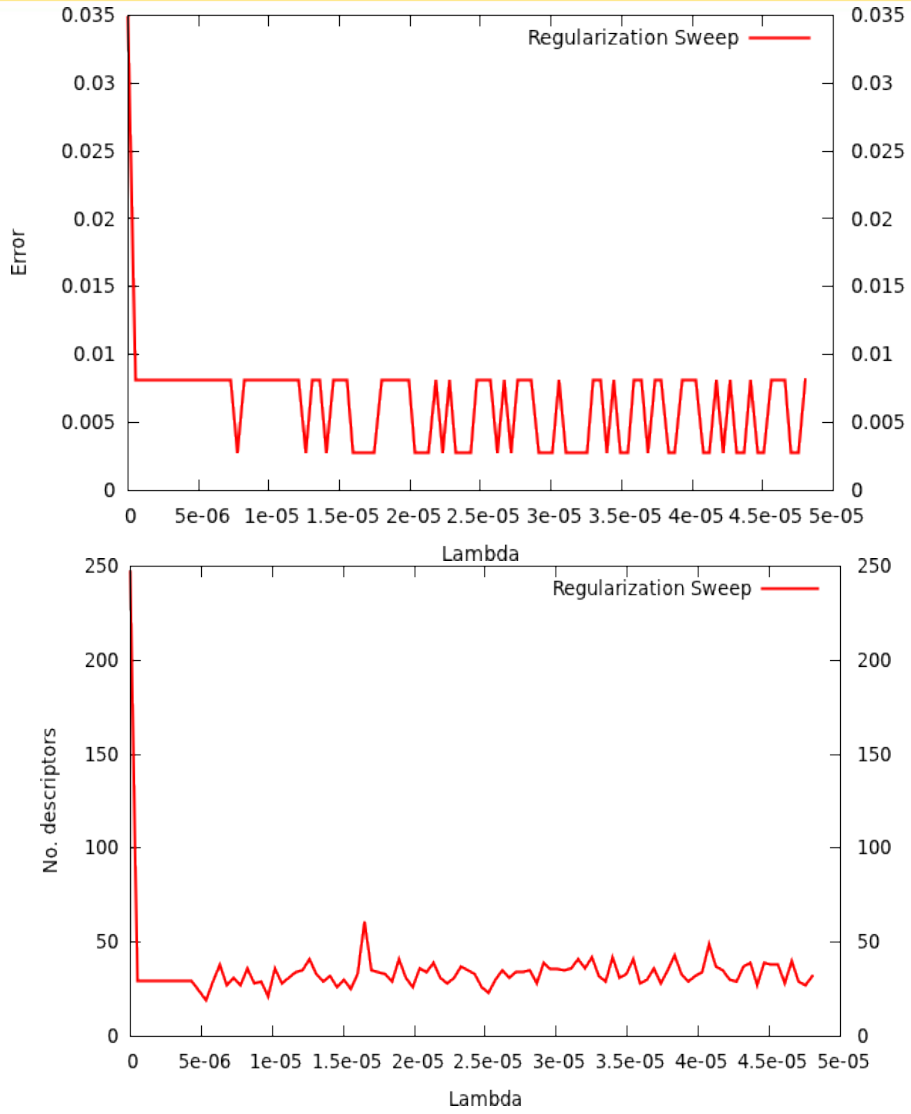


- Even with two descriptor models, weighted errors lower than 10% have been achieved
- Recurring descriptors:
  - Burden matrix - eigenvalues and spectral diameter
  - Moran autocorrelations

USC Viterbi School of Engineering

CEP ML Tests

Information Sciences Institute



$$\sum_{s=1}^{S} H[-y_s Q_w(x_s)] + \lambda \|w\|_0$$

- At small λ, we see the switch from no regularization (200 descriptors) to around 40
- The first points have same error and no. of descriptors. Afterwards, the solution is very degenerate

USC Viterbi School of Engineering

CEP ML Tests

Information Sciences Institute

Lambda	No. descriptors	Wrong	Error
0	247	3	0.034847
4.85E-07	29	3	0.008152
9.70E-07	29	3	0.008152
1.46E-06	29	3	0.008152
1.94E-06	29	3	0.008152
2.43E-06	29	3	0.008152
2.91E-06	29	3	0.008152
3.40E-06	29	3	0.008152
3.88E-06	29	3	0.008152
4.37E-06	29	3	0.008152

- Starting from ~600 Dragon descriptors
- Adding regularization decreases no. of descriptors dramatically
- First few set of lambda values give a similar set of solutions

USC Viterbi School of Engineering

CEP ML Tests

ISI Information Sciences Institute

- **K-fold cross validation:** Data set is divided into *k* subsets, and the holdout method is repeated *k* times

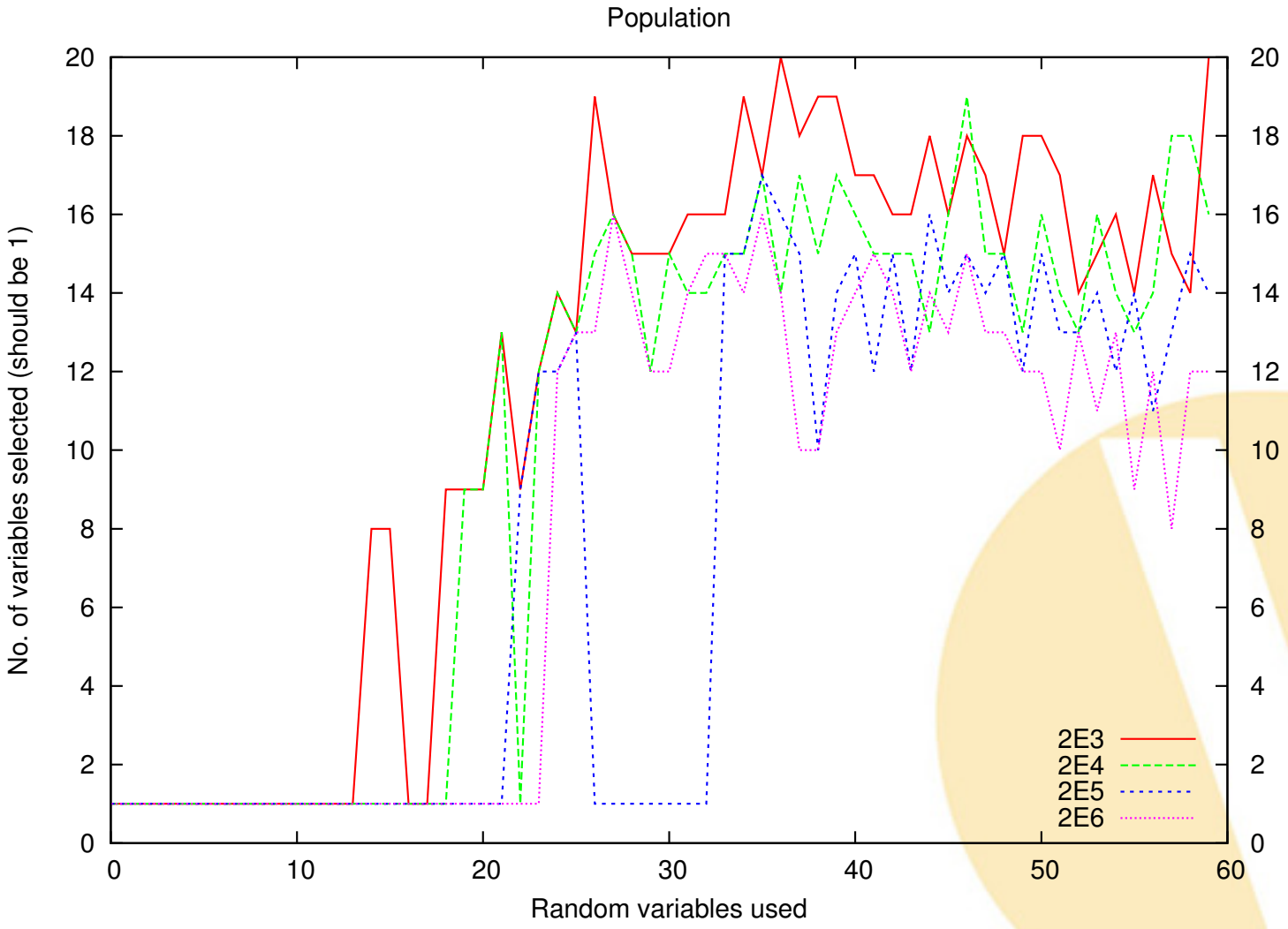
5-fold cross validation using Dragon descriptors					
*k*th	Desc.	Train wrong	Train Error	Val wrong	Val Error
1	11	2	0.006711	5	0.071429
2	16	0	0	0	0
3	18	1	0.003401	0	0
4	12	1	0.003401	2	0.027027
5	12	0	0	0	0
		Average	**0.0047572**		**0.0164456**

- Validation error is slightly higher
- Variation with respect to molecules; Smaller amount of descriptors

USC Viterbi School of Engineering

Test with (mostly) random noise

Information Sciences Institute



USC Viterbi School of Engineering

QUBO and Boosting

Information Sciences Institute

QUBO

$$\min_{\omega} \quad \omega^T Q \omega$$

$$Q_{jj} = -\text{Corr}(h_j, y) + \lambda \qquad Q_{jk} = \frac{\alpha}{2}\text{Corr}(h_j, h_k)$$

Weak class. score — Regularization — Avoid similar class.

$$H(x) = \left(\sum_j \omega_j h_j(x) > T \right)$$

USC Viterbi School of Engineering

QUBO = 2D Random Ising

ISI Information Sciences Institute

$$H_{\text{Ising}} = Q_{jj} Z_j + Q_{jk} Z_j Z_k$$

$$H(s) = (1-s) \sum X_j + s H_{\text{Ising}}$$

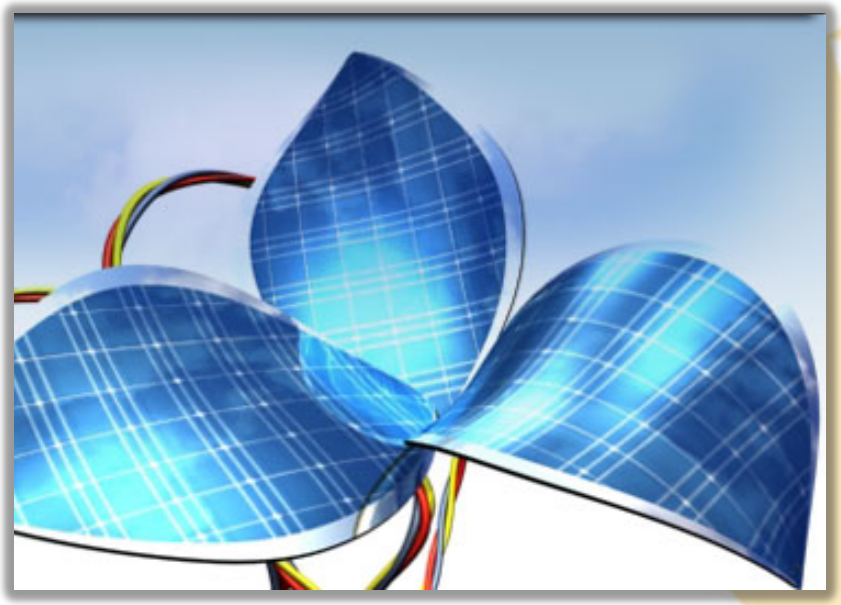
- Can be implemented with D-Wave's chip
- Fairly complicated problems can be addressed
- Approximate solutions are OK (**embedding**)
- Better solutions or potential speedup?
- The final result gives a classical function (Gaussian process)

USC Viterbi School of Engineering

CEP

ISI Information Sciences Institute

- Harvard Clean Energy Project (Alán Aspuru-Guzik et. al.)
- Distributed computing project ("screensaver")
- IBM World Community Grid
- Approximately three years in the making: June 2010 Linux code, November 2010 Windows and Mac codes
- Preliminary results first published: August 2011



USC Viterbi
School of Engineering

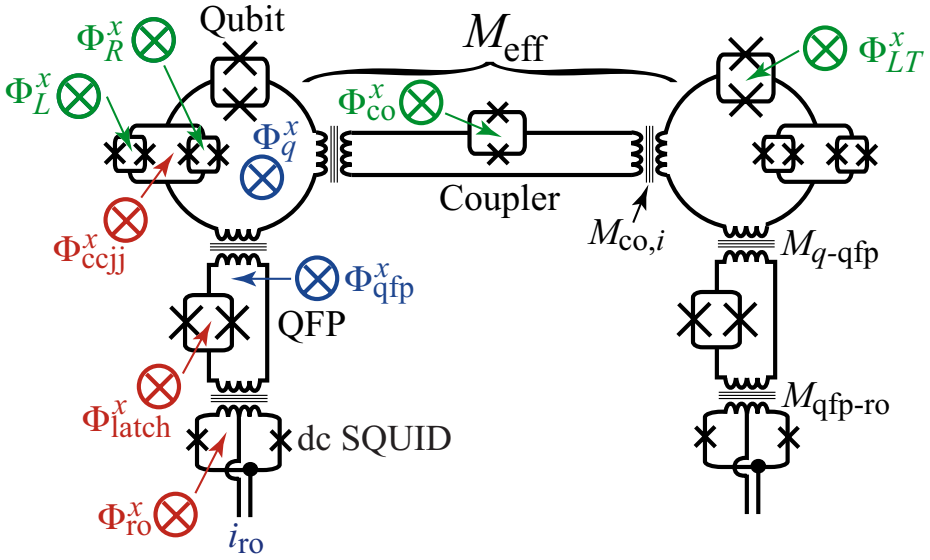
ISI
Information Sciences Institute

Entanglement with fast dephasing adiabatic computation

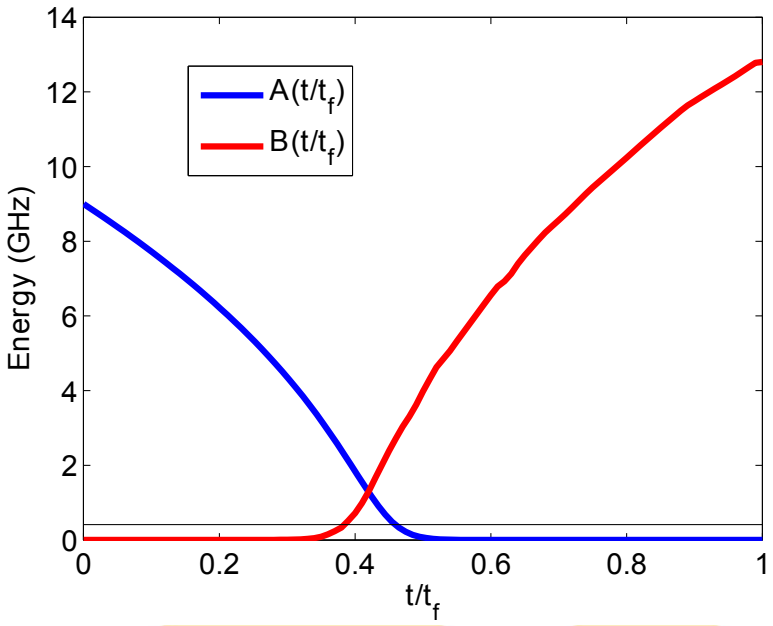
USC Viterbi School of Engineering

D-Wave Qubits

ISI Information Sciences Institute



(a



R. Harris et al., "Experimental demonstration of a robust and scalable flux qubit," Physical Review B, vol. 81, Apr. 2010.

USC Viterbi School of Engineering

Redfield Simulation

ISI Information Sciences Institute

- Energies in GHz range (ns)
- Dephasing (in instantaneous eigenbasis) of around 10ns
- Fast thermalization
- Redfield simulation code provided by M. Amin (R. Harris)
- No concurrence between pairs of qubits (?)

USC Viterbi School of Engineering

PPT Symmetric Extensions

ISI Information Sciences Institute

A state $\tilde{\rho}$ in $\mathcal{H}_A^{\otimes k} \otimes \mathcal{H}_B$ is a PPTSE of ρ in $\mathcal{H}_A \otimes \mathcal{H}_B$ iff

$i)$ $\tilde{\rho}$ is PPT

$ii)$ $\tilde{\rho}$ is invariant under swaps of $\mathcal{H}_A$

$iii)$ $\mathrm{Tr}_{A^{\otimes k-1}}[\tilde{\rho}] = \rho$

All separable states have a PPTSE for any k

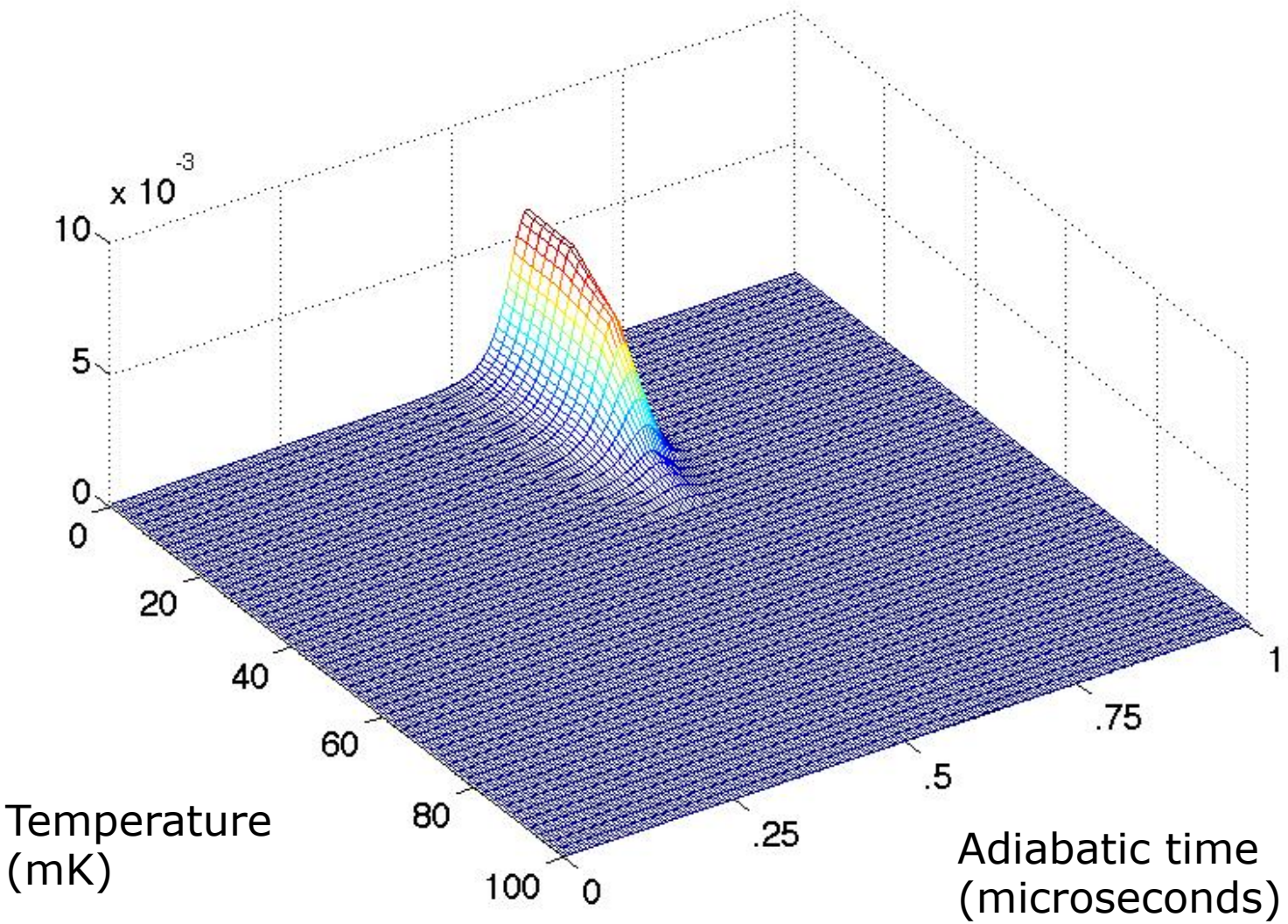
$$\tilde{\rho} = \sum_i p_i |\psi_i\rangle\langle\psi_i|^{\otimes k} \otimes |\phi_i\rangle\langle\phi_i|$$

F. Spedalieri et. al.

USC Viterbi School of Engineering

Witness entanglement

Information Sciences Institute



USC Viterbi
School of Engineering

ISI
Information Sciences Institute

Questions?