Title: Machine learning phase discovery in quantum gas microscope images

Speakers: Ehsan Khatami

Collection: Machine Learning for Quantum Design

Date: July 11, 2019 - 2:00 PM

URL: http://pirsa.org/19070030

Abstract: Site resolution in quantum gas microscopes for ultracold atoms in optical lattices have transformed quantum simulations of many-body Hamiltonians. Statistical analysis of atomic snapshots can produce expectation values for various charge and spin correlation functions and have led to new discoveries for the Hubbard model in two dimensions. Conventional approaches, however, fail in general when the order parameter is not known or when an expected phase has no clear signatures in the density basis. In this talk, I will introduce our efforts in using machine learning techniques to overcome this challenge with snapshots of fermionic atoms. Collaborators: Richard Scalettar (UC Davis), Waseem Bakr (Princeton), and Juan Carrasquilla (Vector Institute)

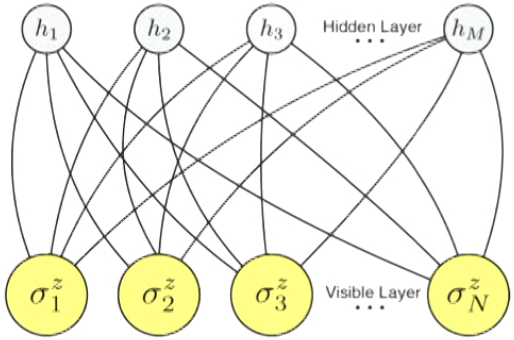
Machine Learning Feature Extraction in Quantum Gas Microscope Images

Ehsan Khatami
San Jose State University

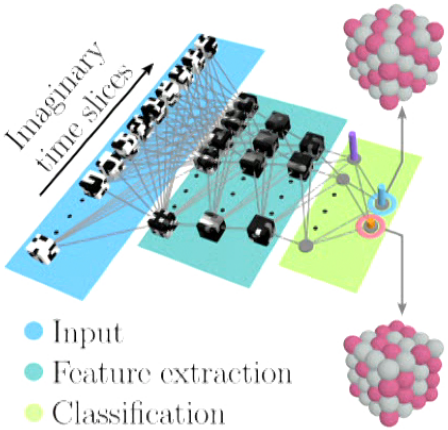
Machine Learning for Quantum Design
Perimeter Institute, July 11, 2019

In collaboration with
Juan Carrasquilla (Vector Inst.)
Richard Scalettar (UC Davis)
Waseem Bakr (Princeton)

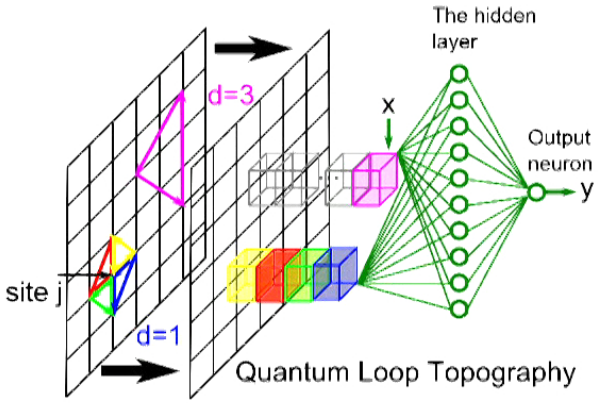
Machine Learning for Quantum Many-Body Physics



G. Carleo and M. Troyer,
Science **355**, 602 (2017)

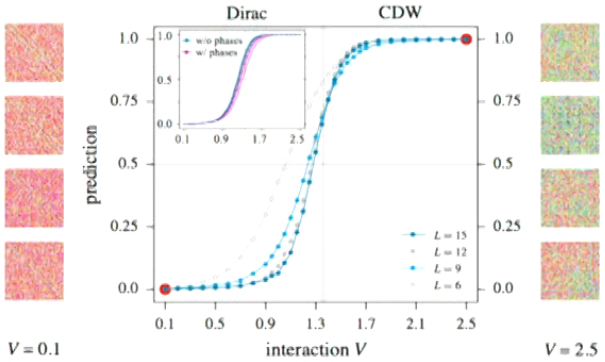


K. Ch'ng, J. Carrasquilla, R. G. Melko, EK,
PRX **7**, 031038 (2017)

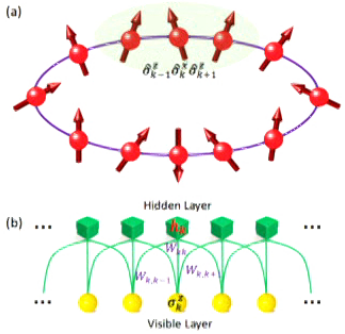


Y. Zhang, E. Kim,
PRL **118**, 216401 (2017)

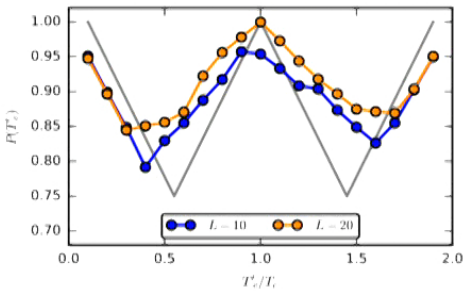
K. Ch'ng, N. Vazquez, EK, PRE **97**, 013306 (2018)



P. Broecker, J. Carrasquilla, R. G. Melko & S. Trebst
Scientific Reports **7**, 8823 (2017)



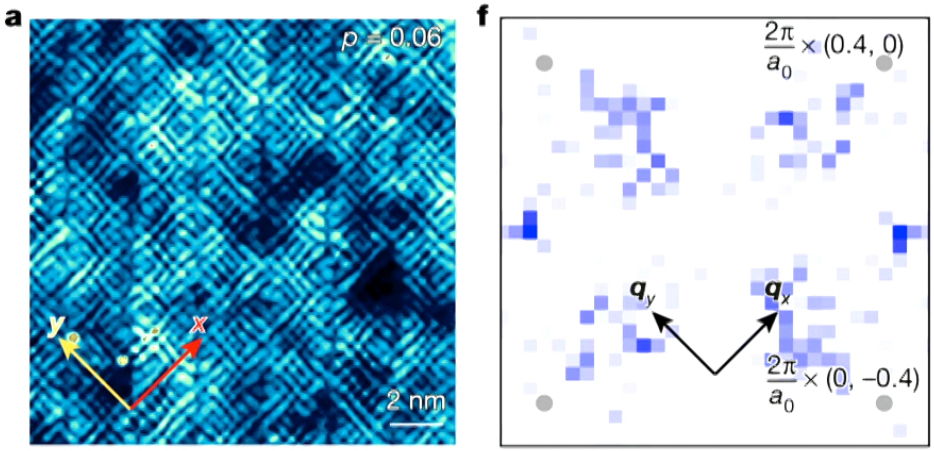
Dong-Ling Deng,
Xiaopeng Li, and
S. Das Sarma,
Phys. Rev. B **96**,
195145 (2017)



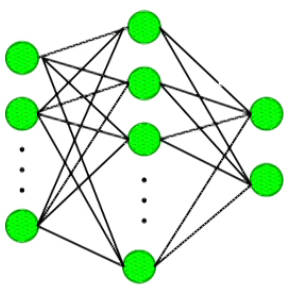
Evert P.L. van Nieuwenburg, Ye-Hua Liu, and Sebastian D. Huber,
Nat. Phys. **13**, 435 (2017)

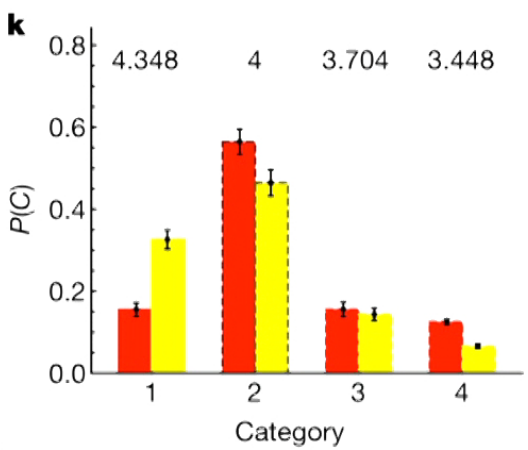
And many more …

Machine Learning and Experiments

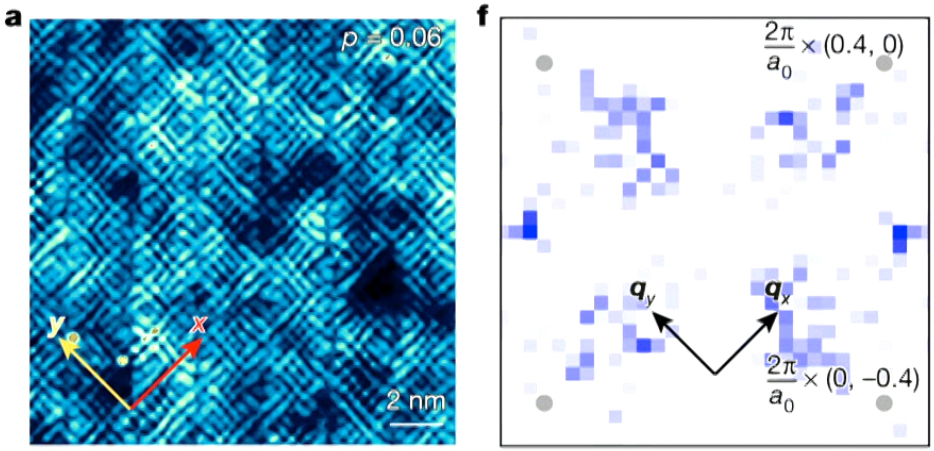


Zhang et al., Nature **570**, 484 (2019)





Machine Learning and Experiments



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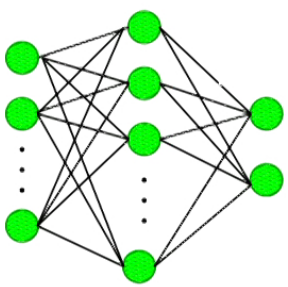
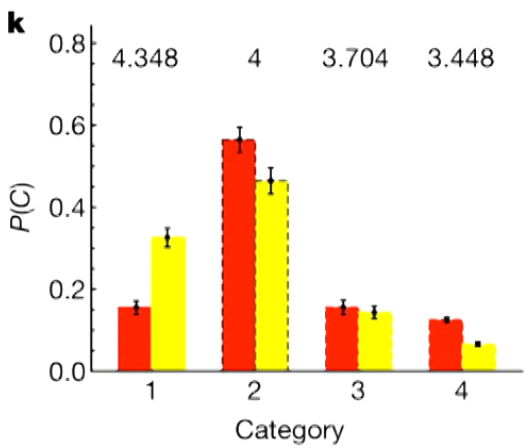
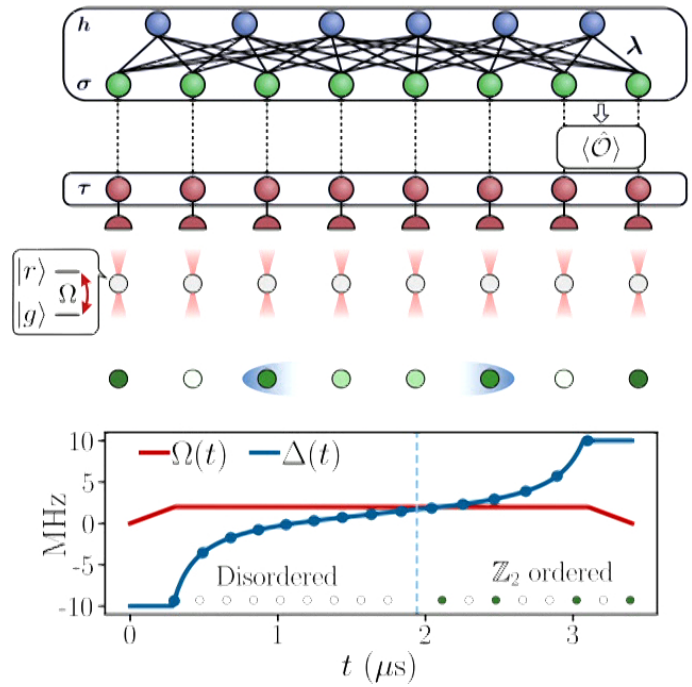






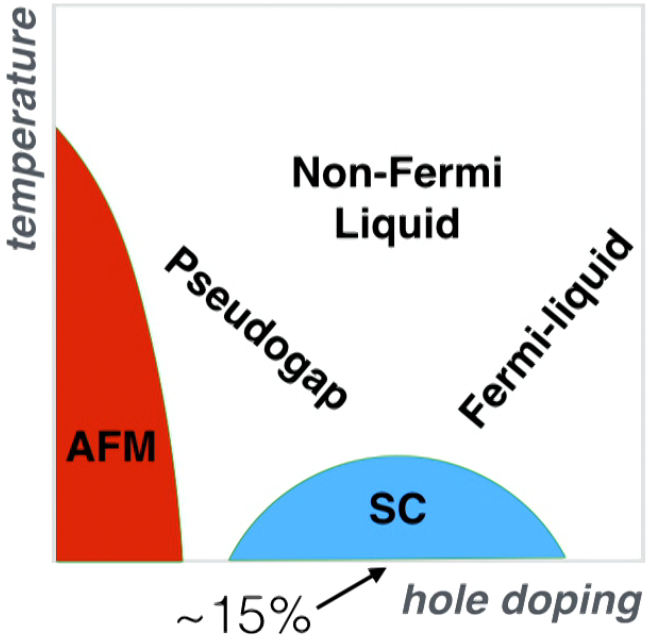
Torlai et al., arXiv:1904.08441

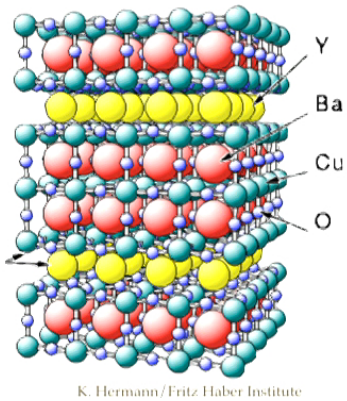
Few other applications:
L. R. B. Picard, M. J. Mark, F. Ferlaino, R. van Bijnen, arXiv:1904.08074

Wigley et al., Sci. Rep. **6**, 25890 (2016)

Cuprates and the Fermi-Hubbard model

Cartoon of cuprates phase diagram





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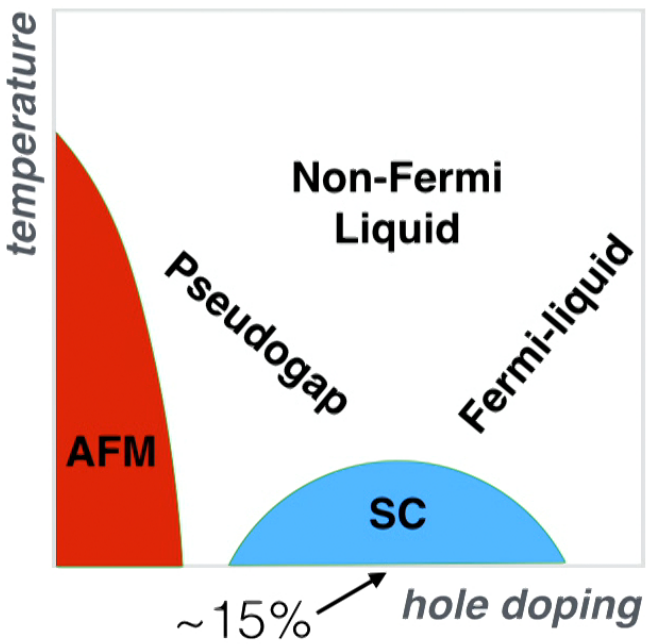
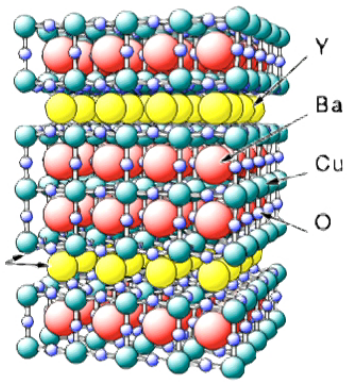
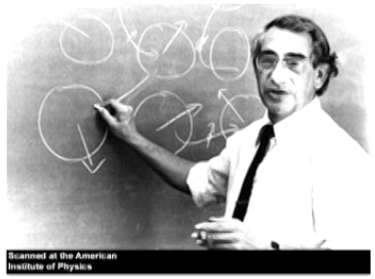




K. Hermann/Fritz Haber Institute

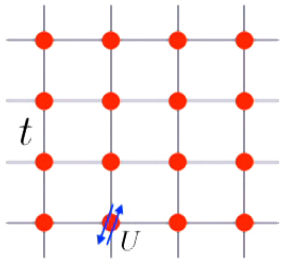
Enrico Fermi

John Hubbard



$$H = t \sum_{\langle ij \rangle \sigma} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

The Fermi-Hubbard model on the square lattice



Optical Lattice Experiments

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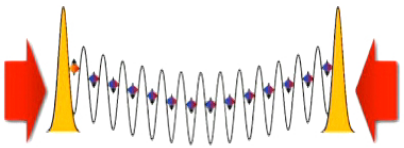

Wang et al., 2014

Optical Lattice Experiments

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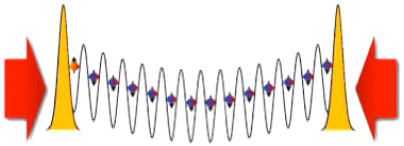
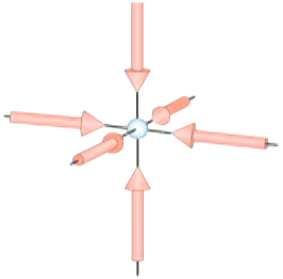
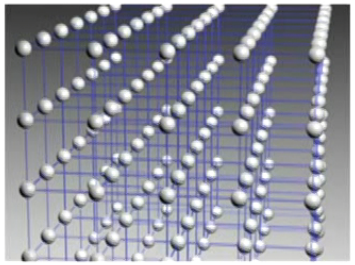


Wang et al., 2014





Bloch's group

Optical Lattice Experiments

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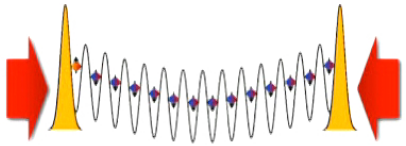
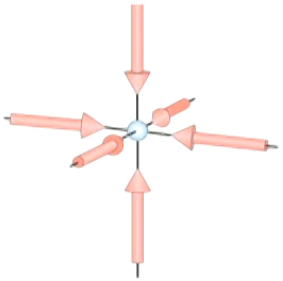
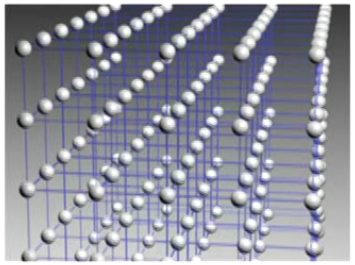


Wang et al., 2014





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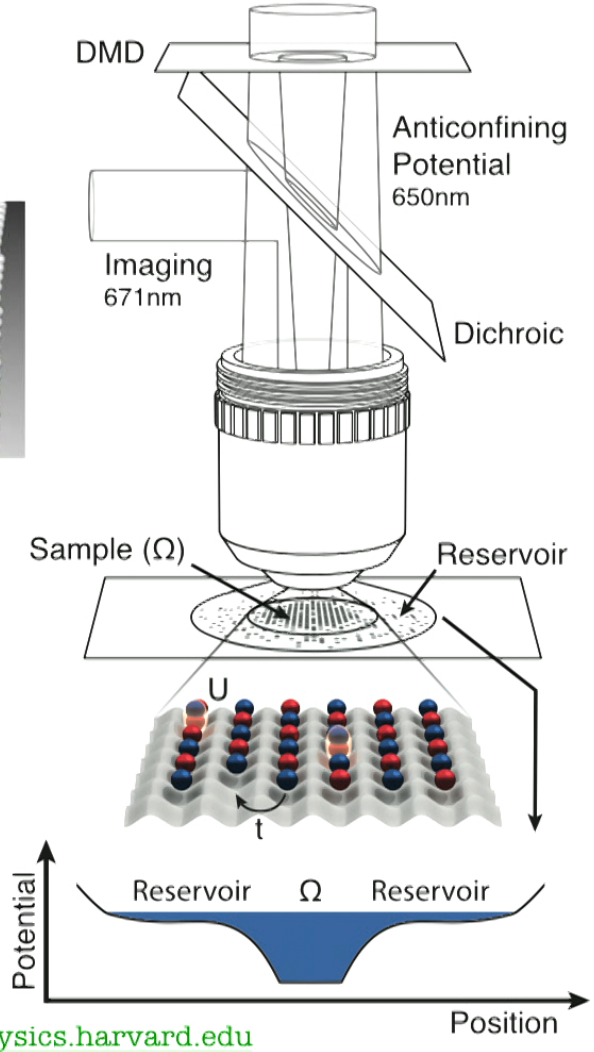

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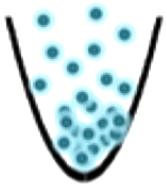
Nature **545**, 462 (2017)

Optical Lattice Experiments



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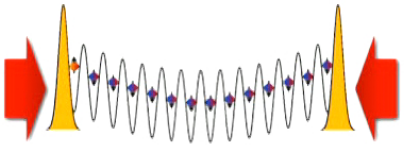
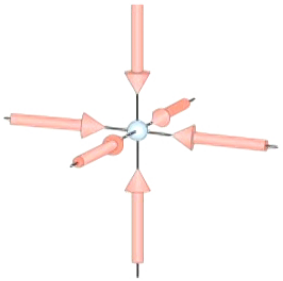
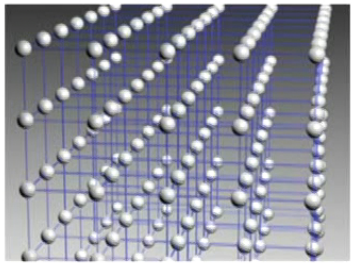


Wang et al., 2014





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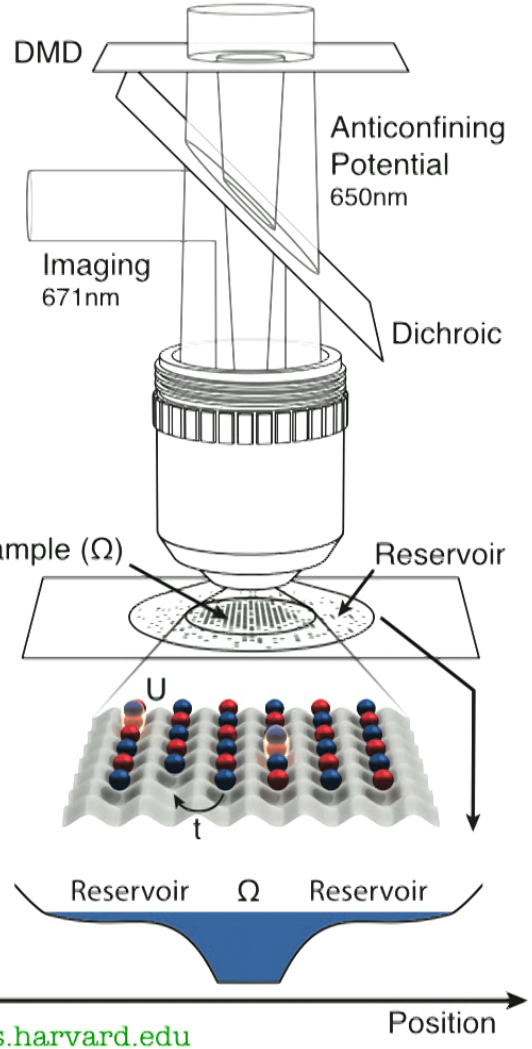

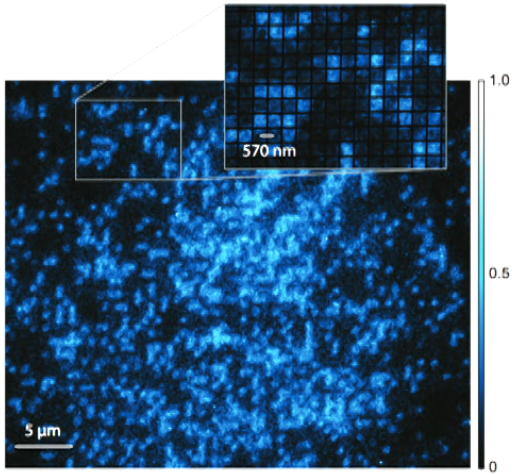

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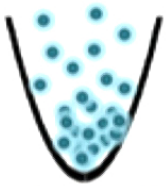
Nature **545**, 462 (2017)

Optical Lattice Experiments



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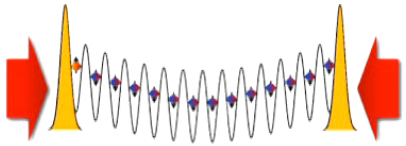
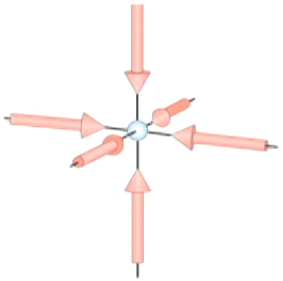
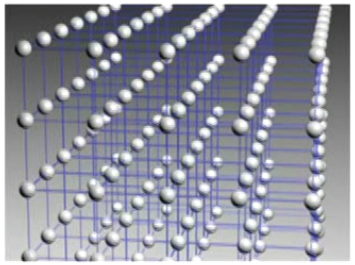


Wang et al., 2014





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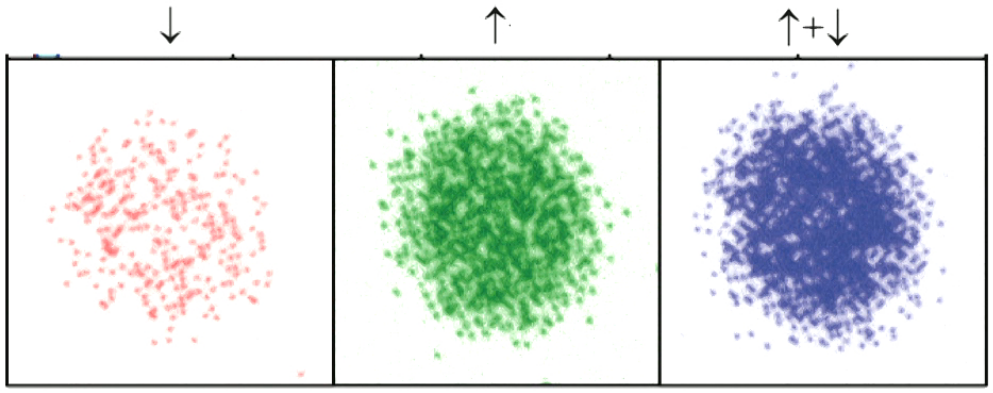
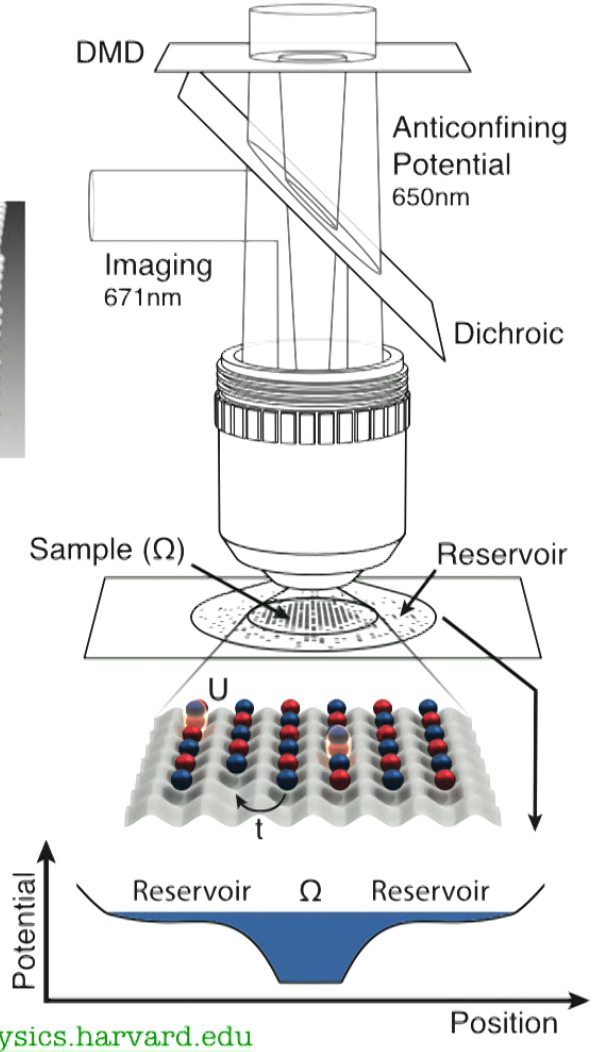


Bakr's group: Science **357**, 1385 (2017)



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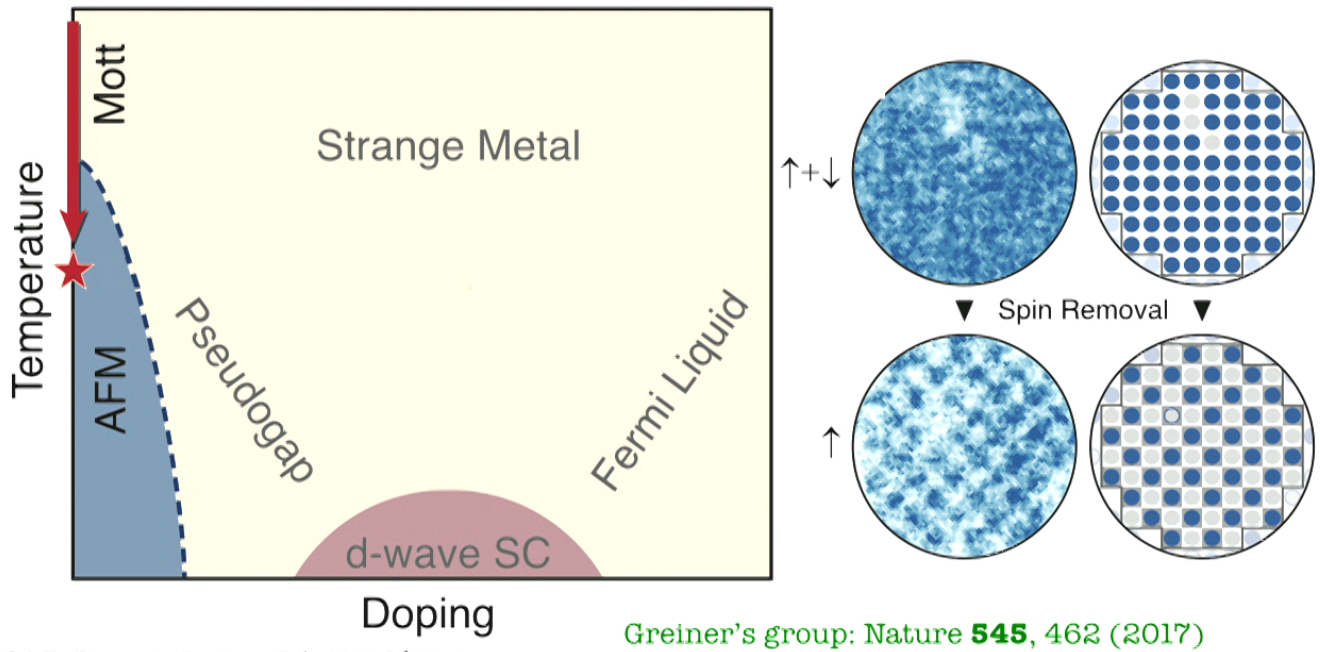
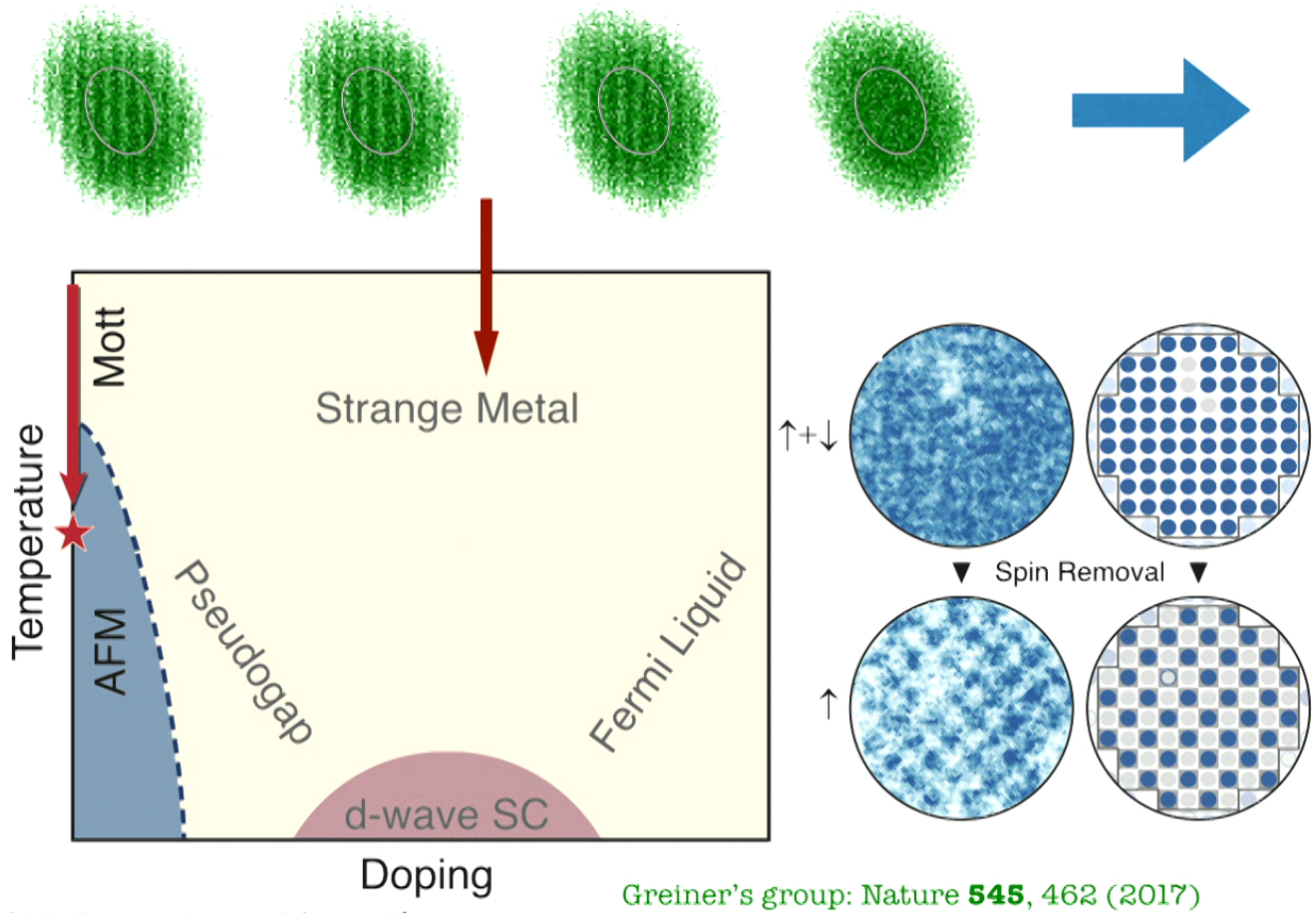
Nature **545**, 462 (2017)

Optical Lattice Experiments

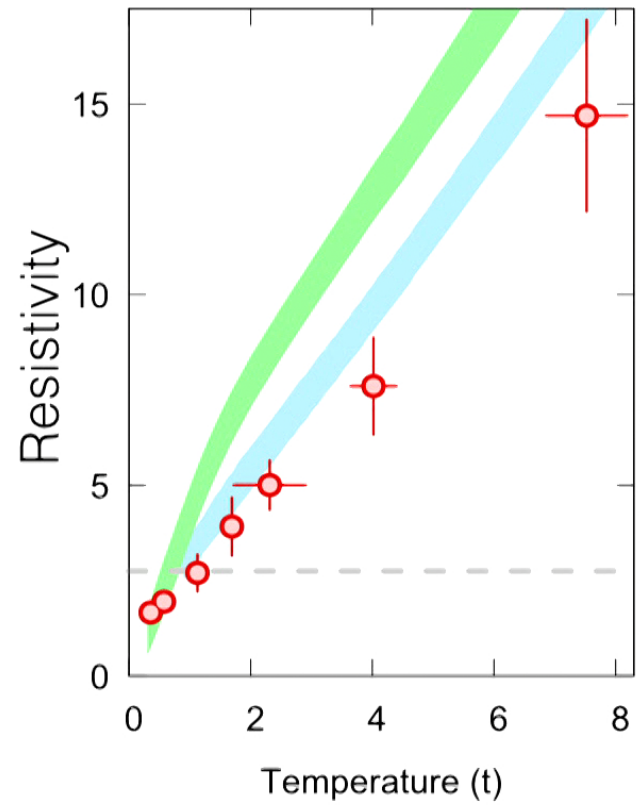


Greiner's group: Nature **545**, 462 (2017)

Optical Lattice Experiments



Greiner's group: Nature **545**, 462 (2017)

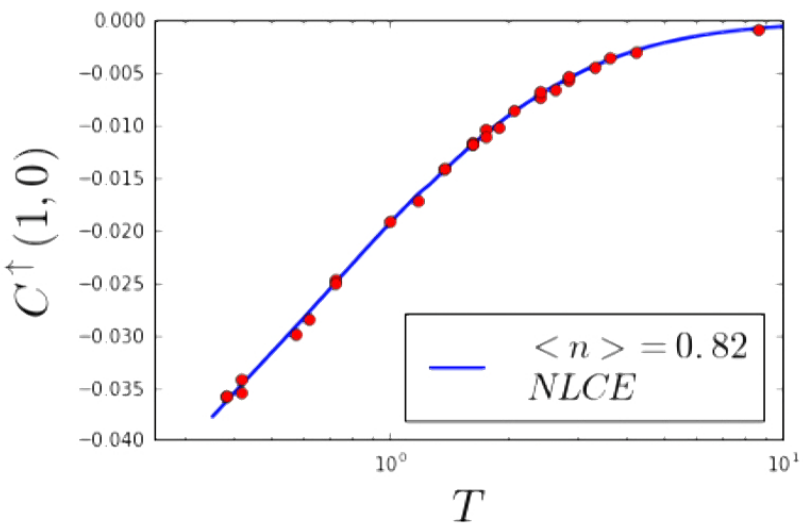


Bakr's group: Science, **363**, 379 (2019)

Also see
Zwierlein's group: Science, **363**, 383 (2019)
for spin conductivity.

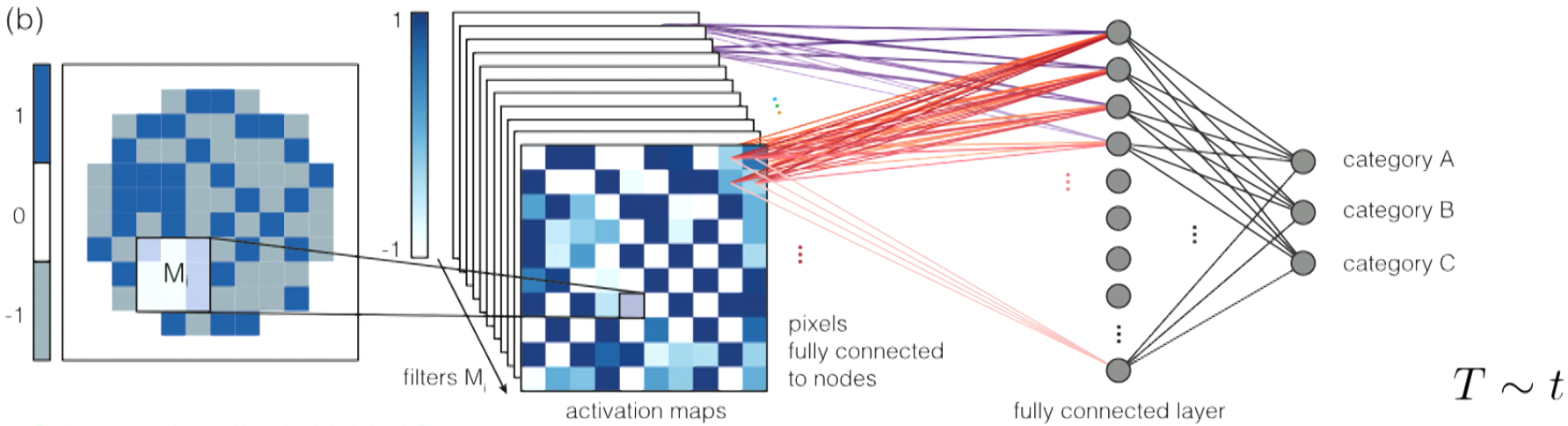
Temperature Estimates

Example:
nearest neighbor spin-up density-density correlation function



Symbols: experiment samples
Line: Numerical linked-cluster expansion

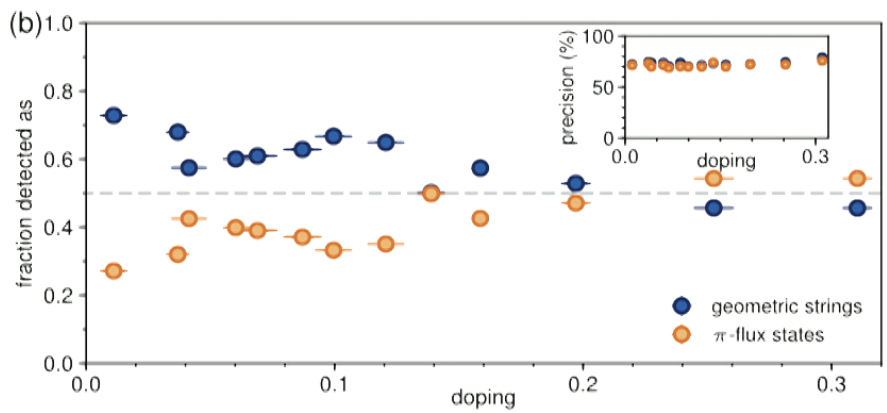
Machines Favoring Theories



$T \sim t$

Bohrdt et al., arXiv:1811.12425

- Train convolutional neural networks on simulated snapshots based on two different theories
- Classify experimental snapshots



Can We Discover New Physics?

- Can we extract features from the experimental snapshots?
- Do phases like the non-Fermi liquid, pseudogap or d-wave superconductivity have any **signatures in the density basis**?
- Can we use theoretical snapshots to guide future experiment?

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Experimental Snapshots

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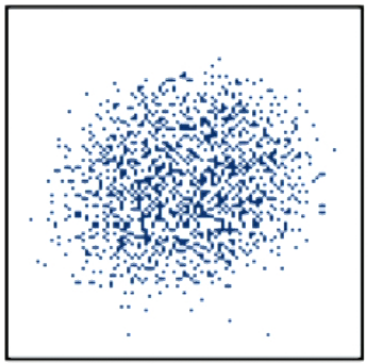
Spin-ups

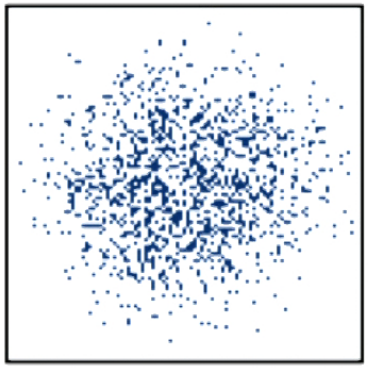
$$\begin{cases} n \sim 0.82 \\ U \sim 7.5t \end{cases}$$

(the "non-Fermi liquid" phase)

T~0.35t



T~7.5t



100×100

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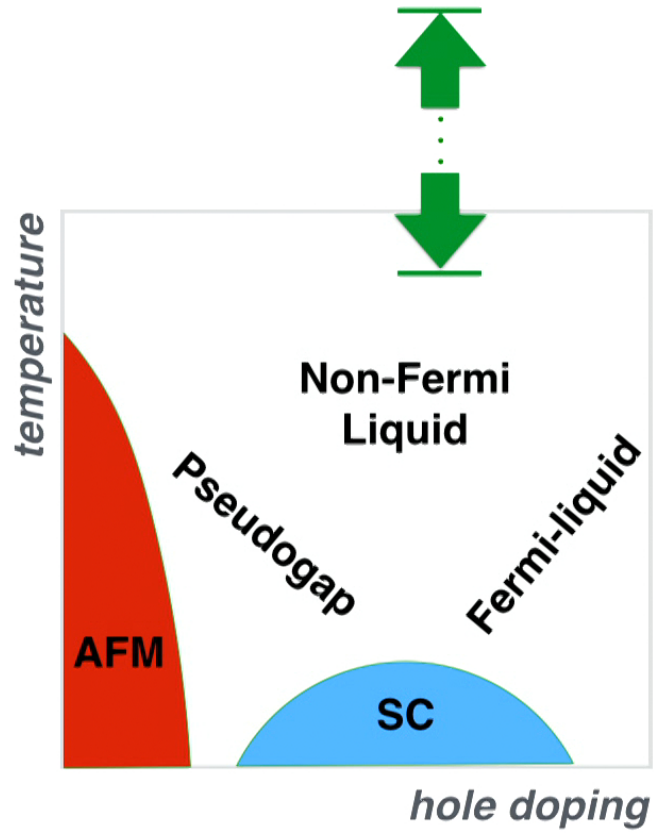

Experimental Snapshots

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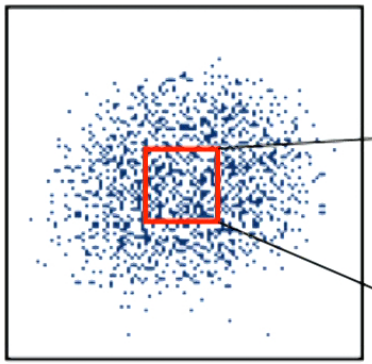
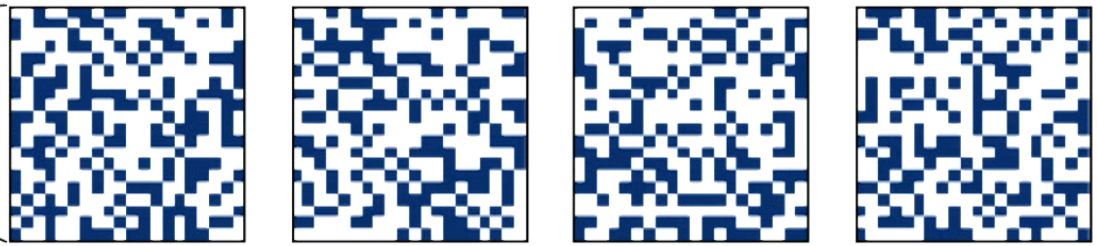


20×20



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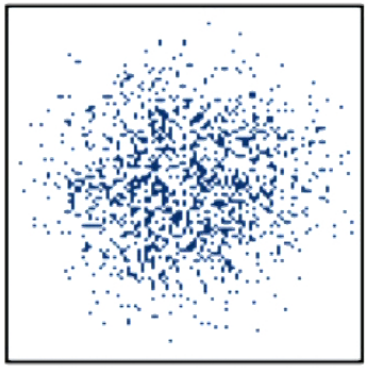
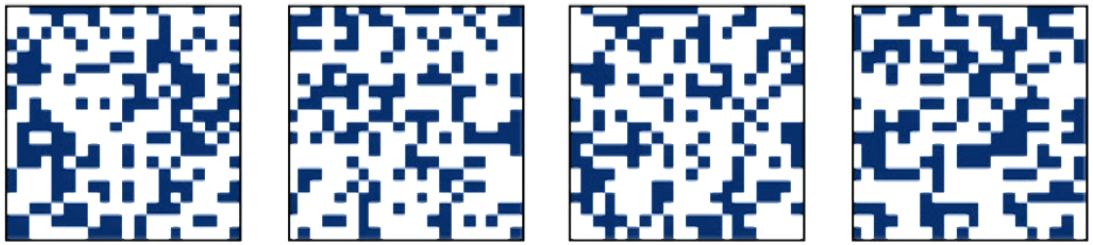
T~7.5t



100×100

$pixels$



. . .

Experimental Snapshots

sites.ualberta.ca/~ljleblan/

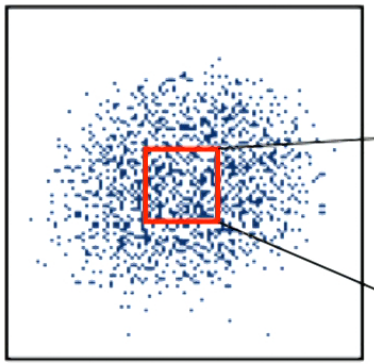
Spin-ups

$$\begin{cases} n \sim 0.82 \\ U \sim 7.5t \end{cases}$$

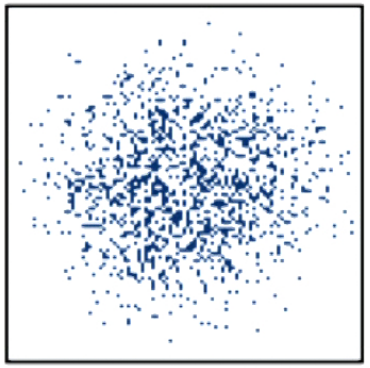
(the "non-Fermi liquid" phase)

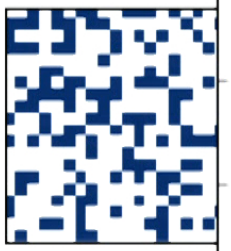
T~0.35t

T~7.5t



20×20





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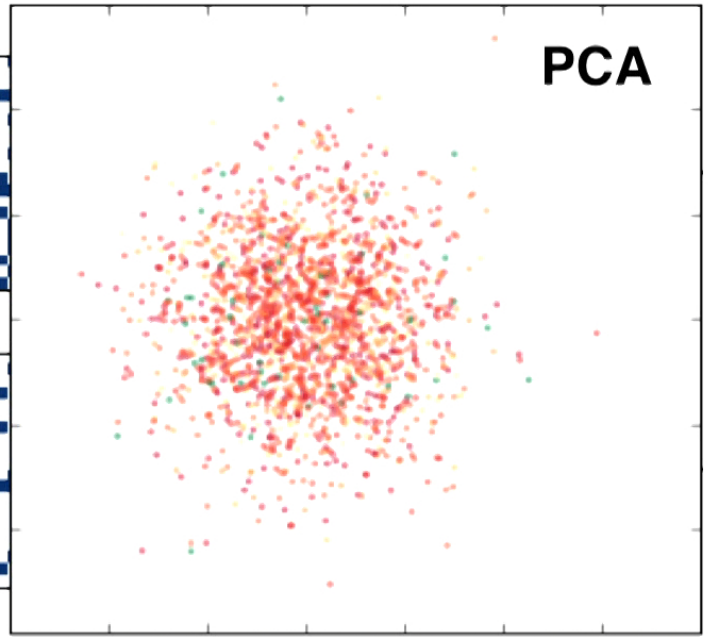
pixels



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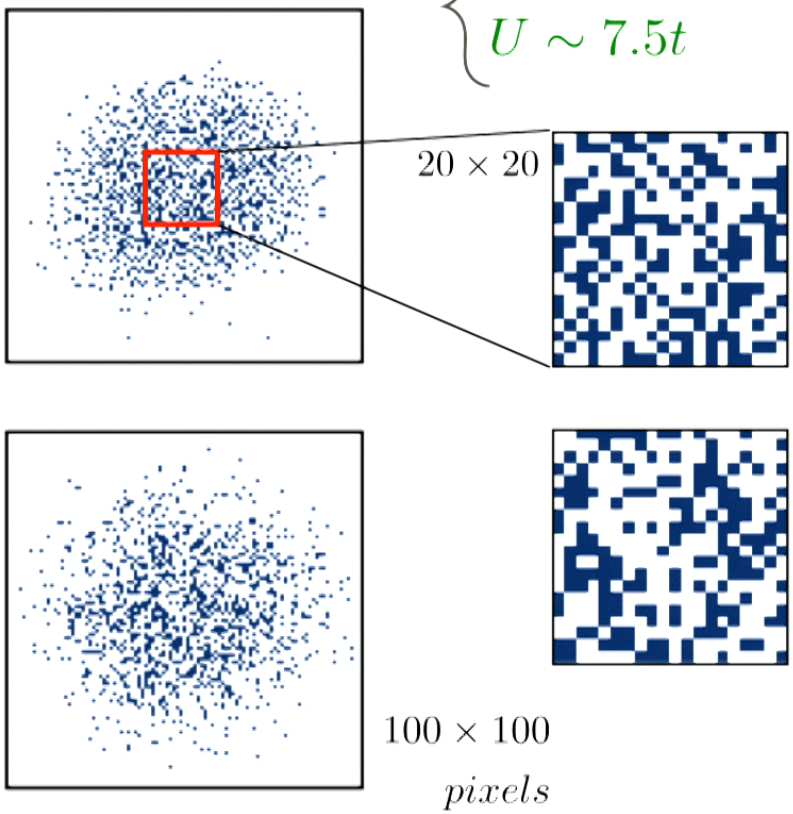
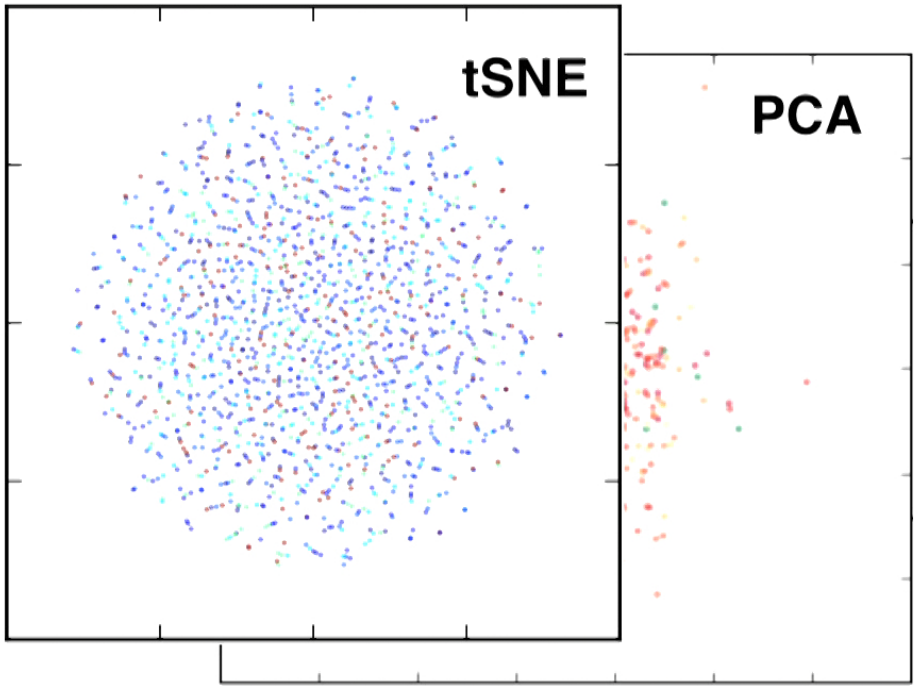
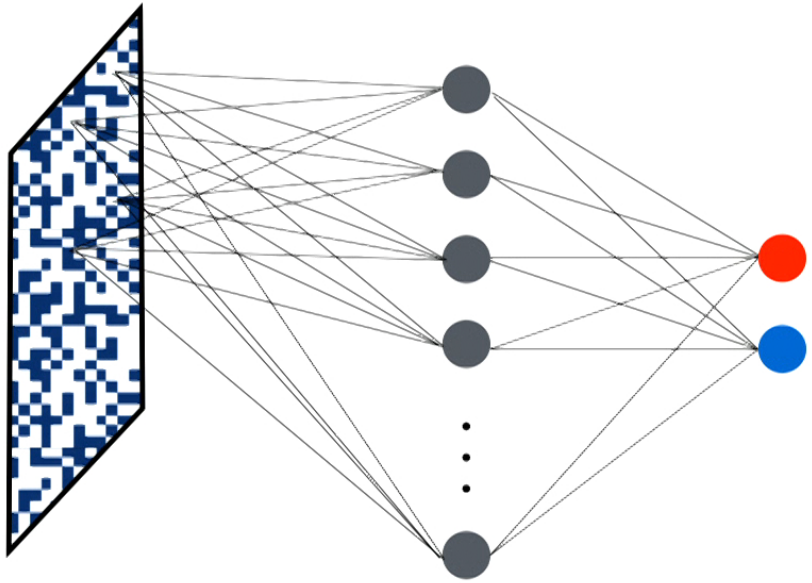


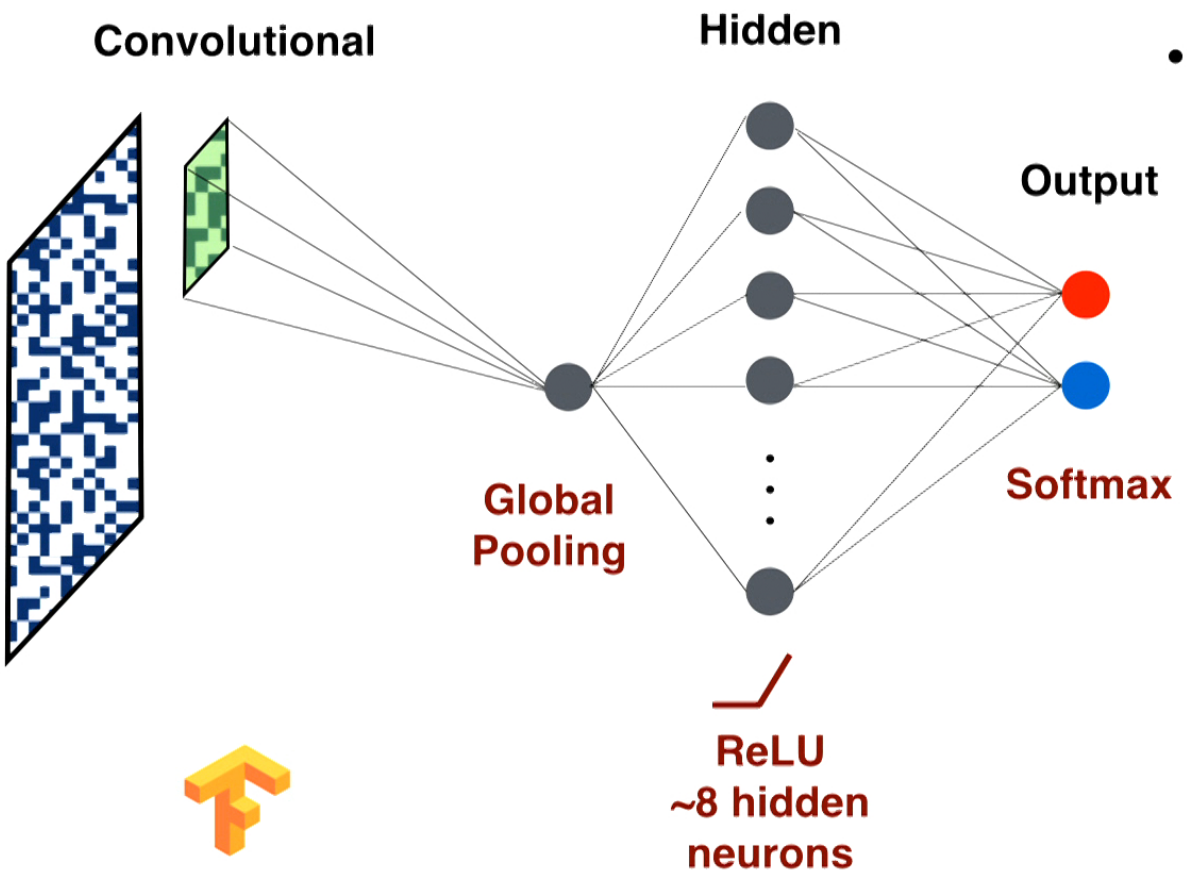


Artificial Neural Networks

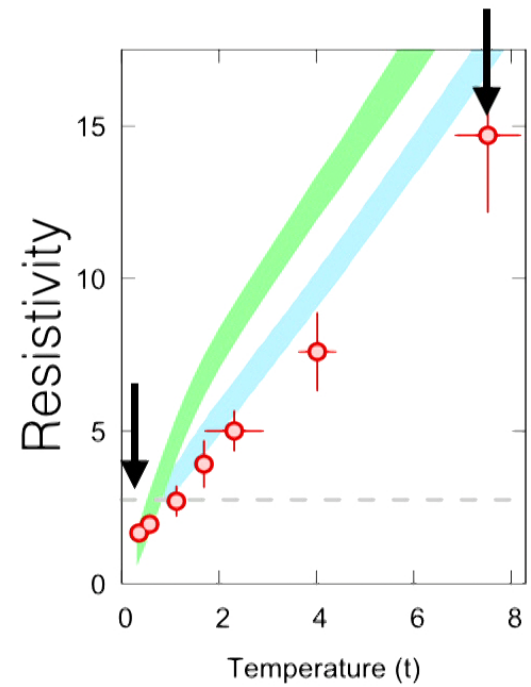


- Artificial neural networks are usually opaque.
- However, one can try to extract features if convolutional layers are used.

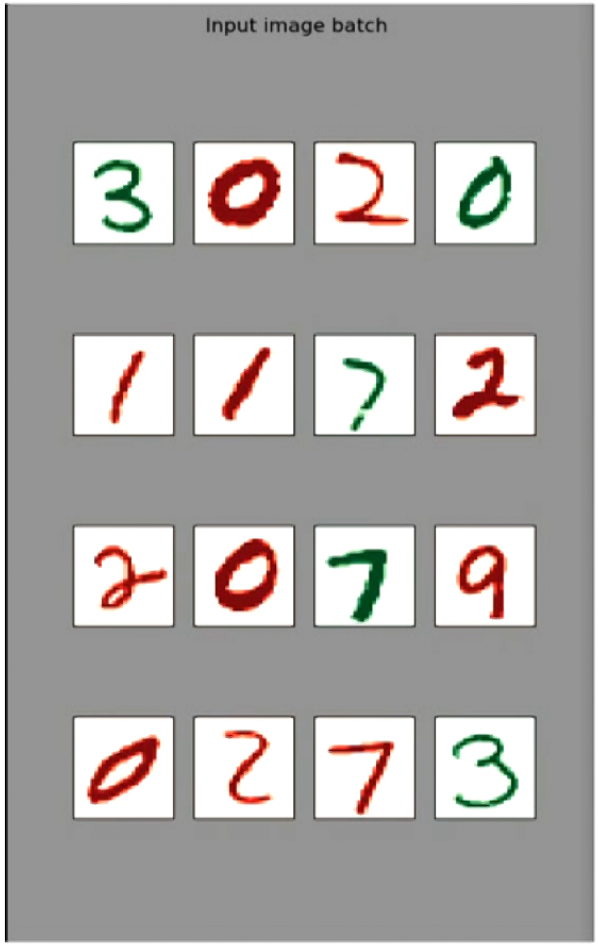
Convolutional Neural Networks

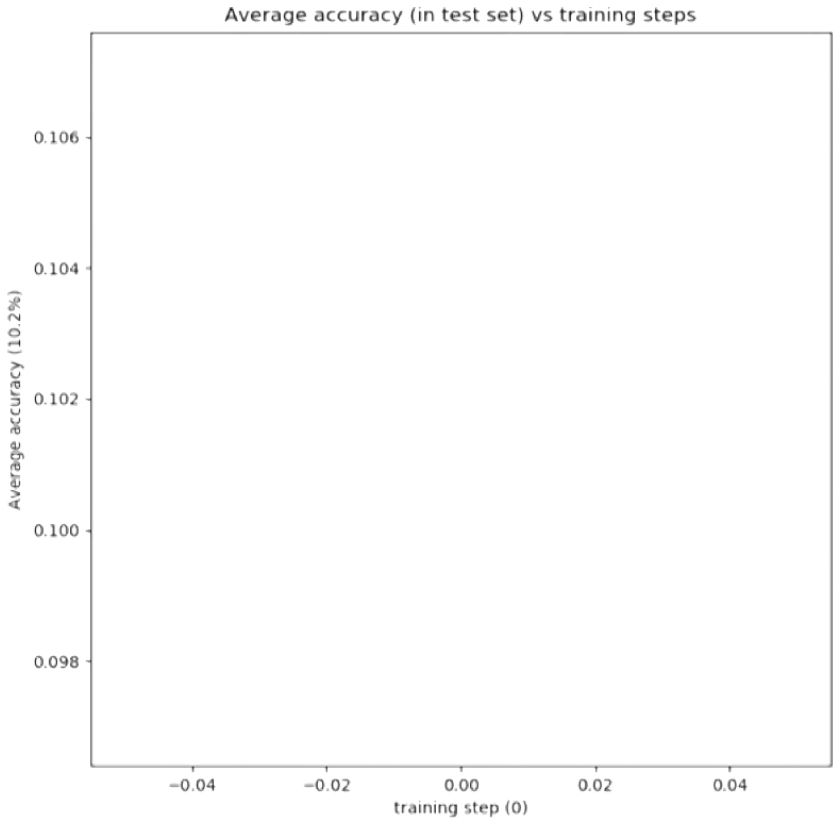


- Train using snapshots at the extreme temperatures.



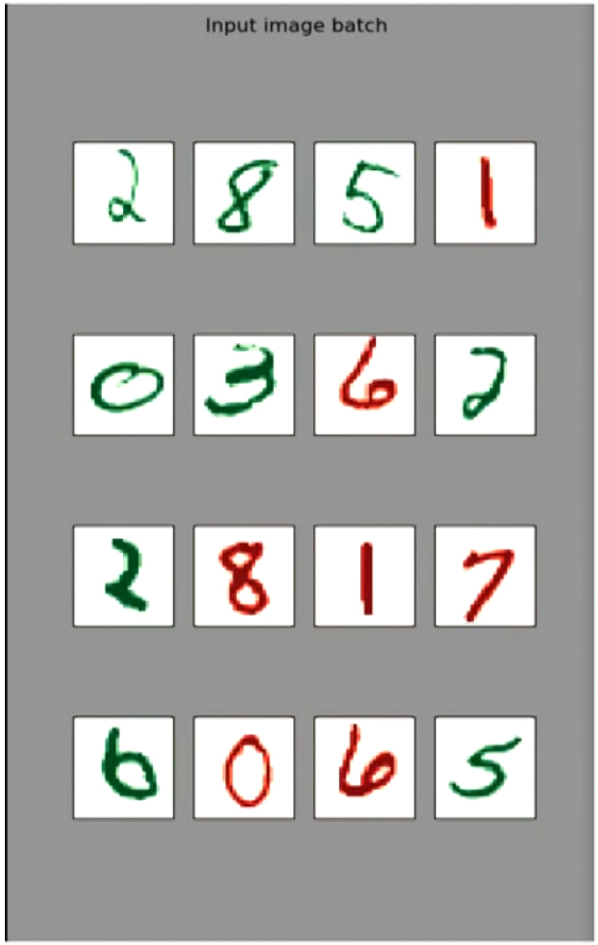
Feature Extraction

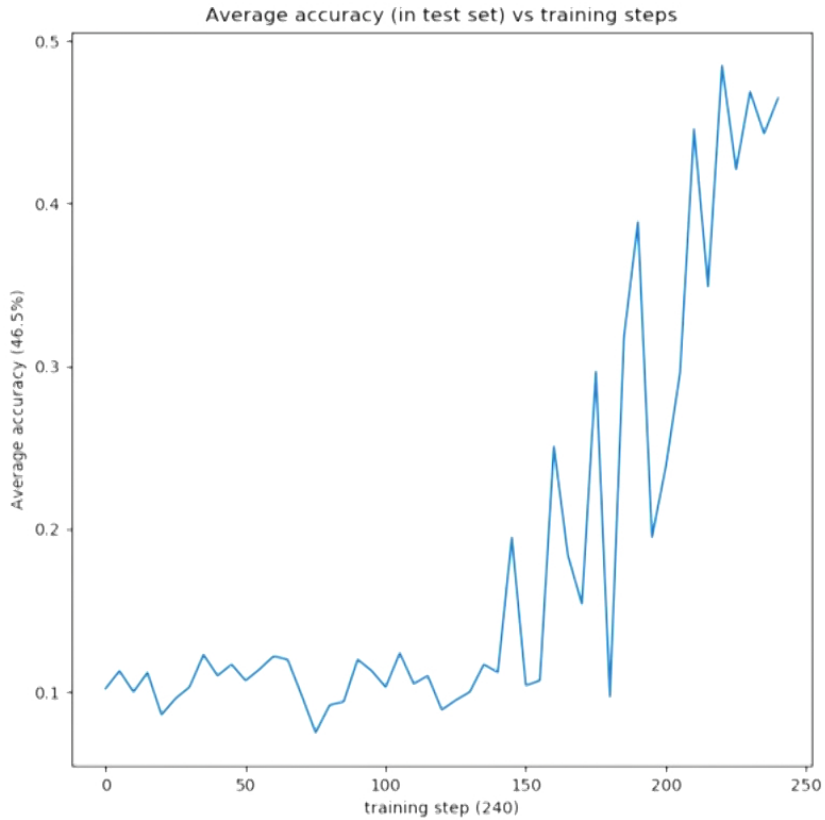


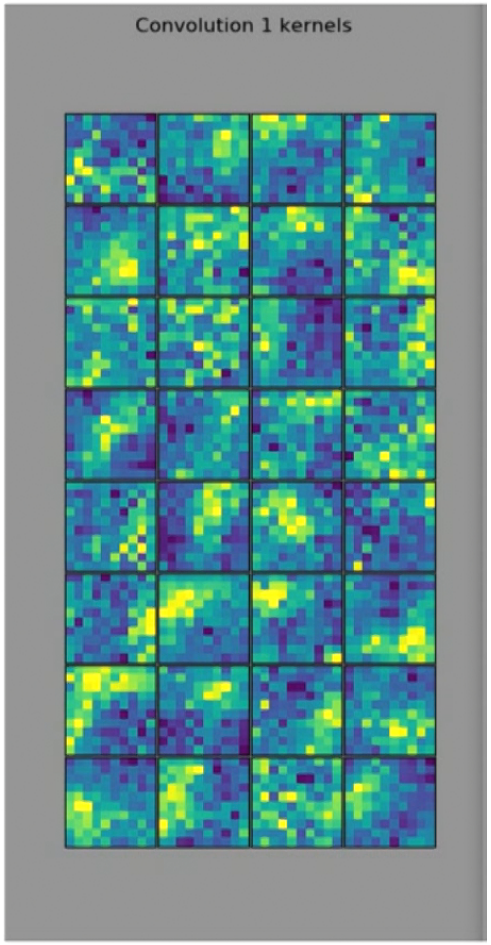


https://www.youtube.com/watch?v=VUkFo6IXMJc

Feature Extraction







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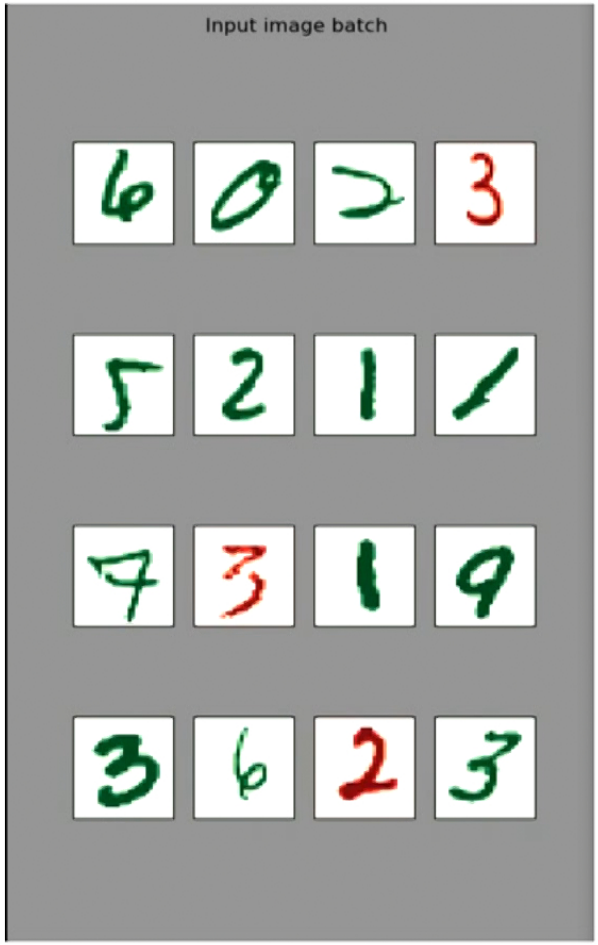
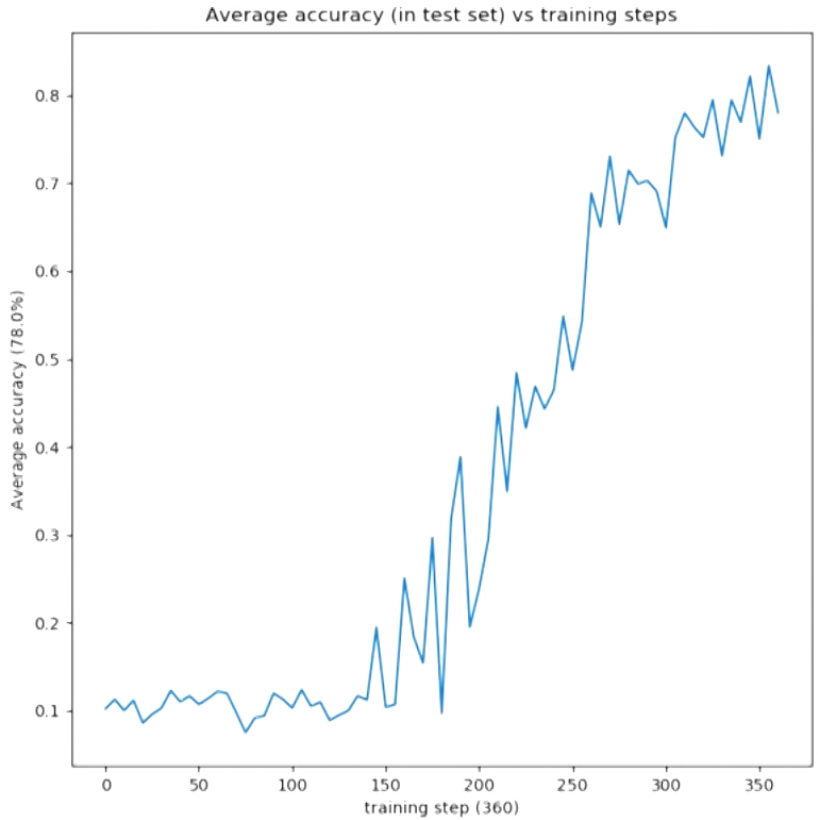
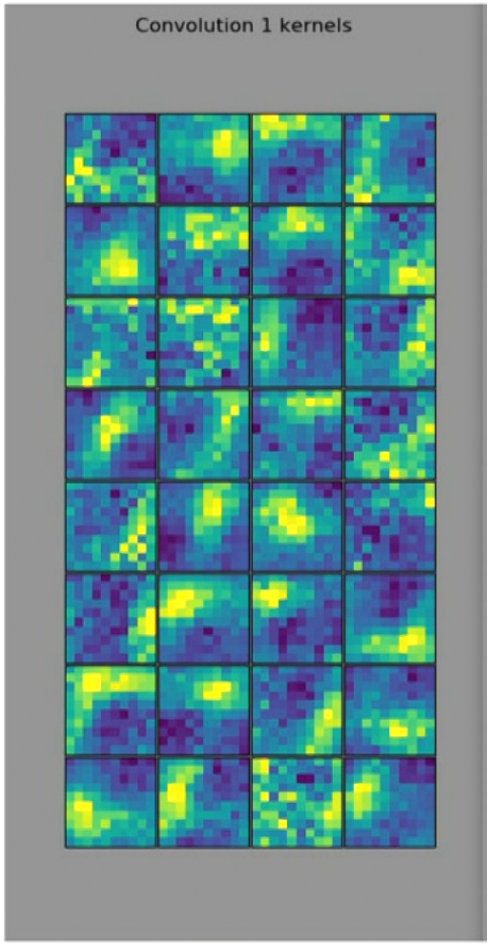
Feature Extraction







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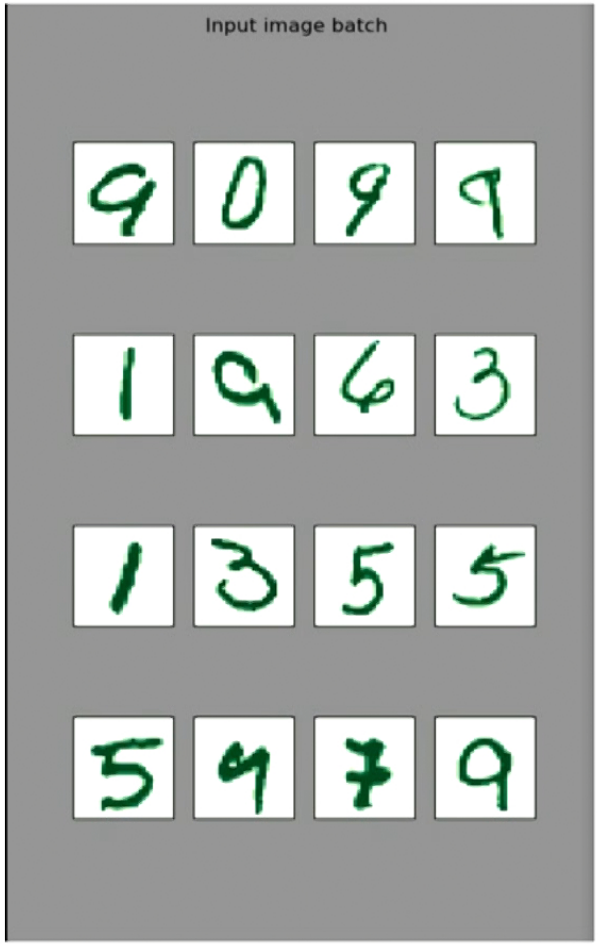

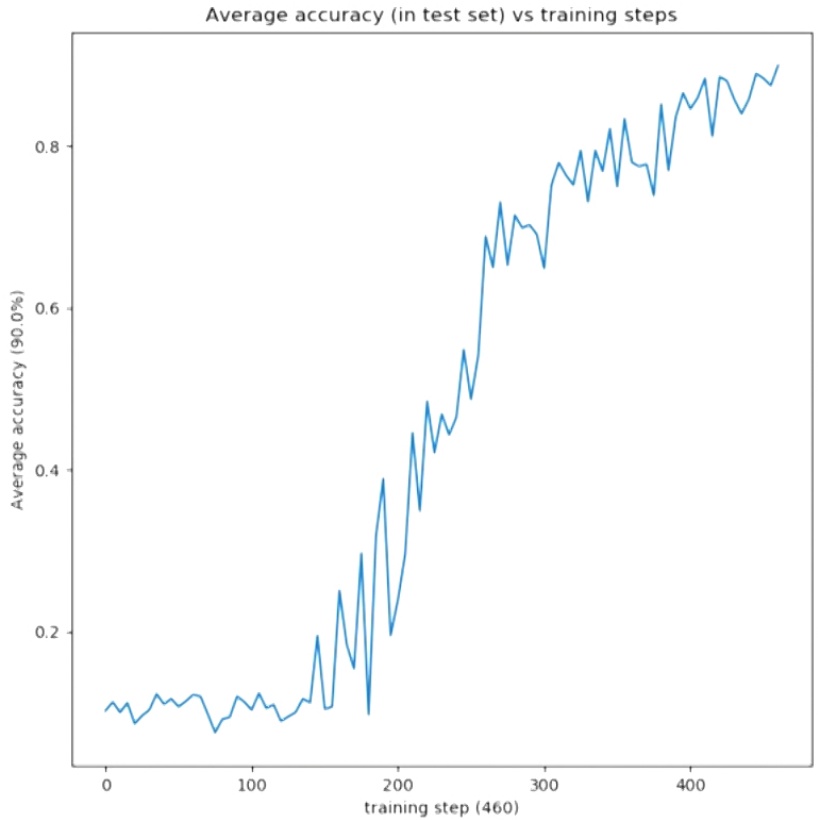

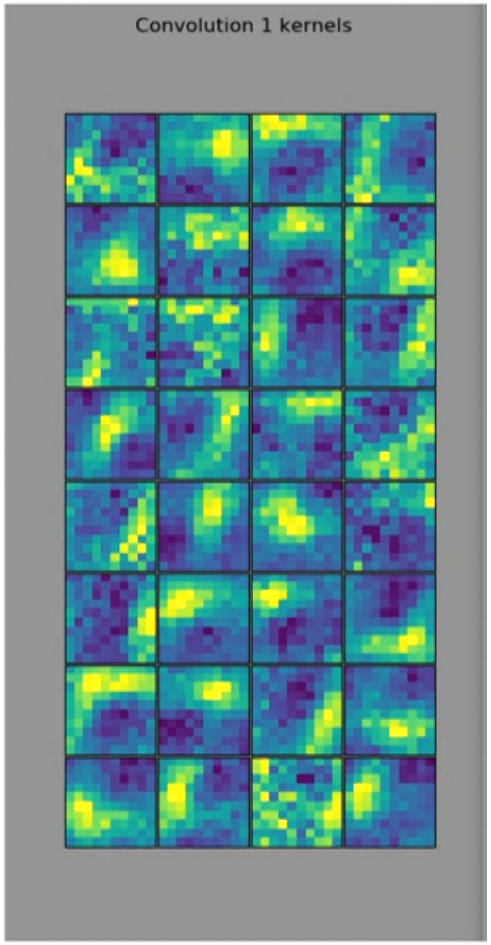

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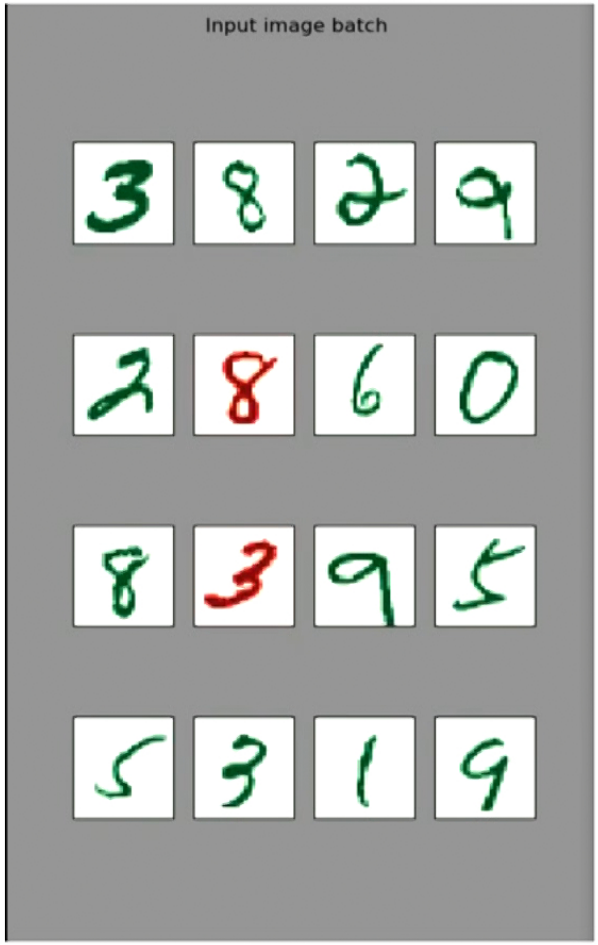
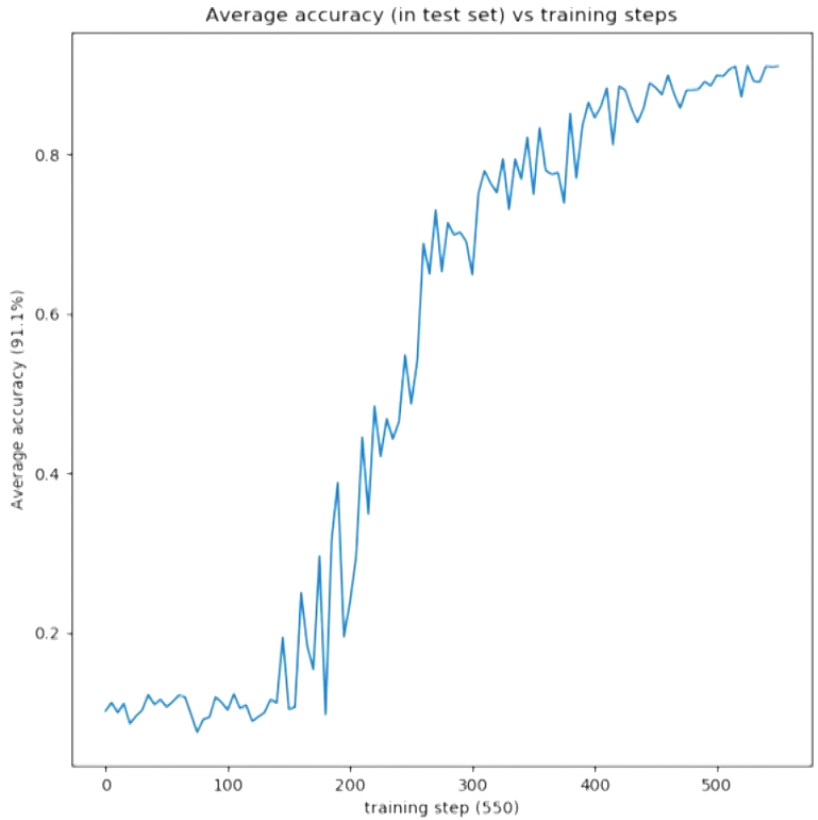
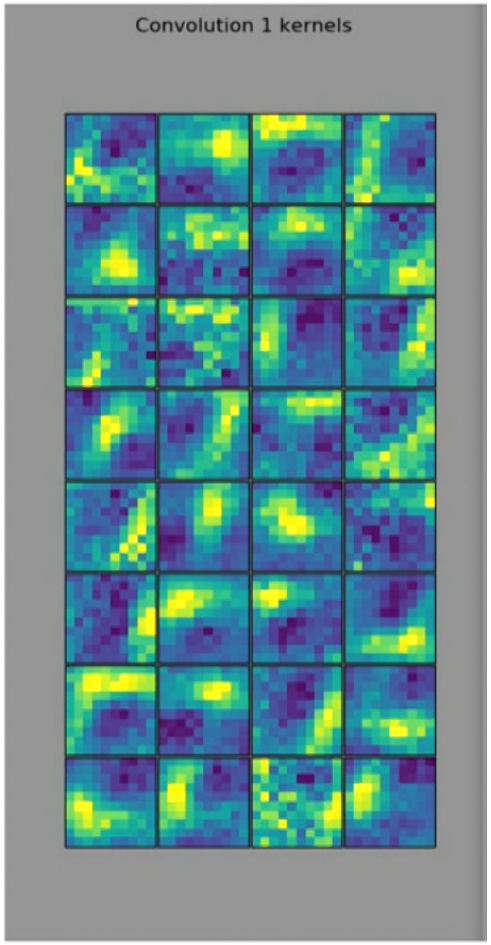
Feature Extraction







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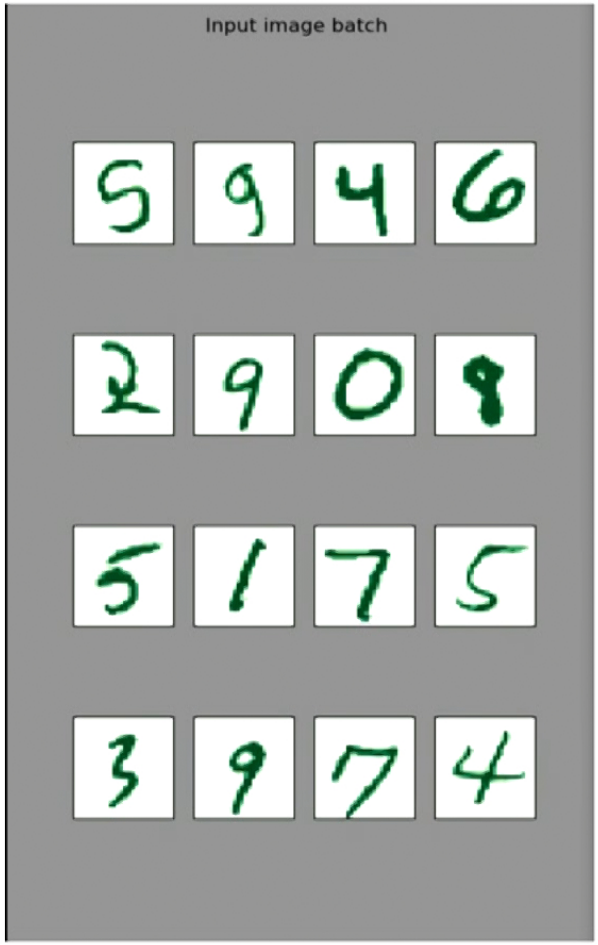
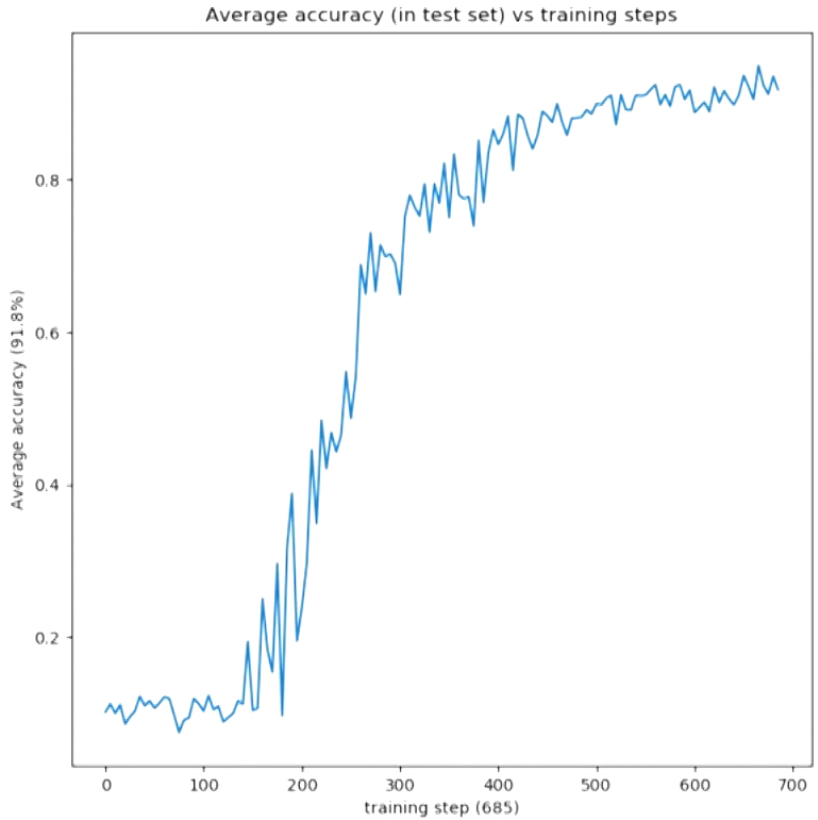
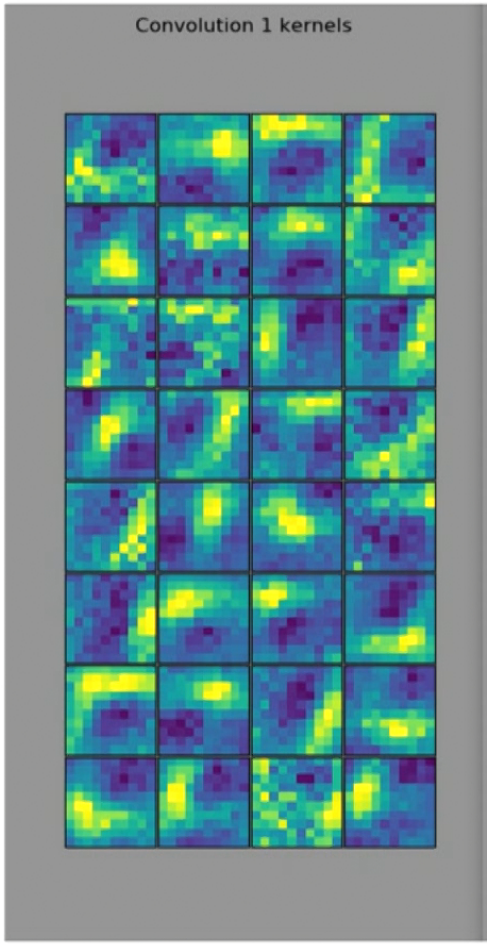
Feature Extraction





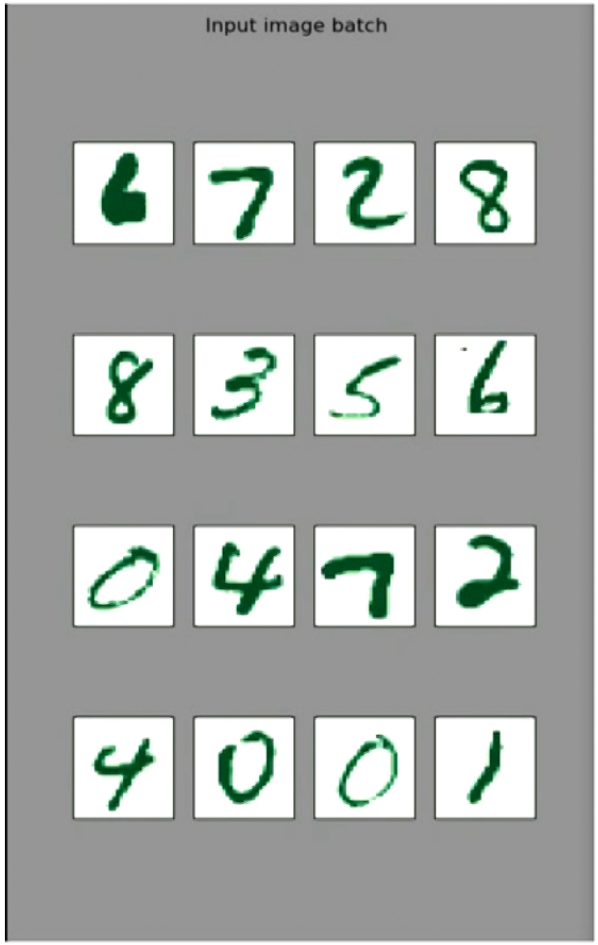


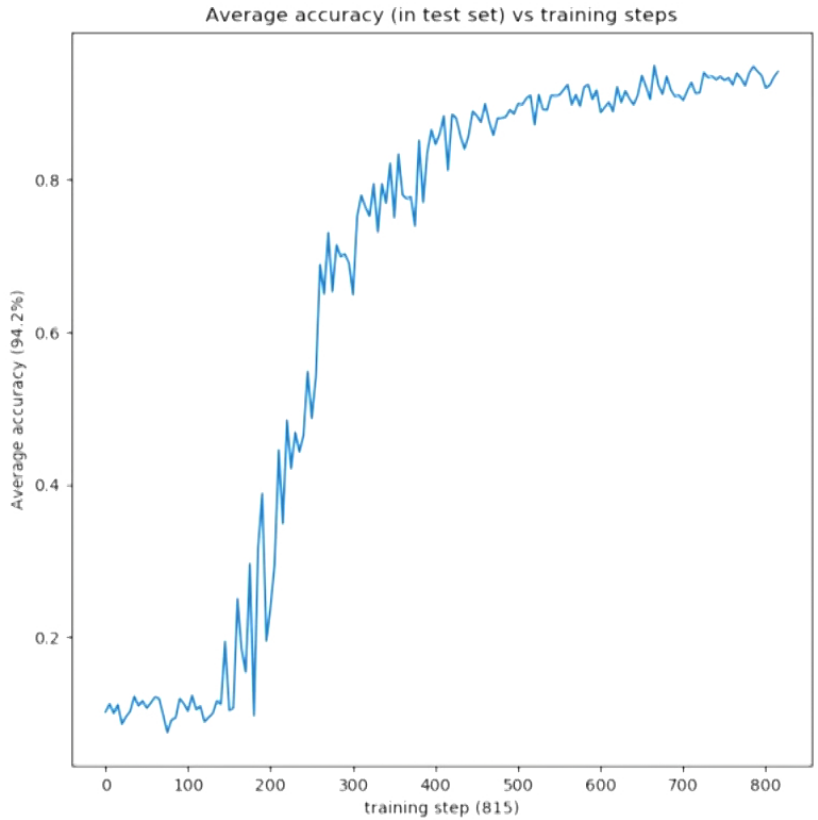
Q ML, Perimeter Institute, July 2019, Khatami

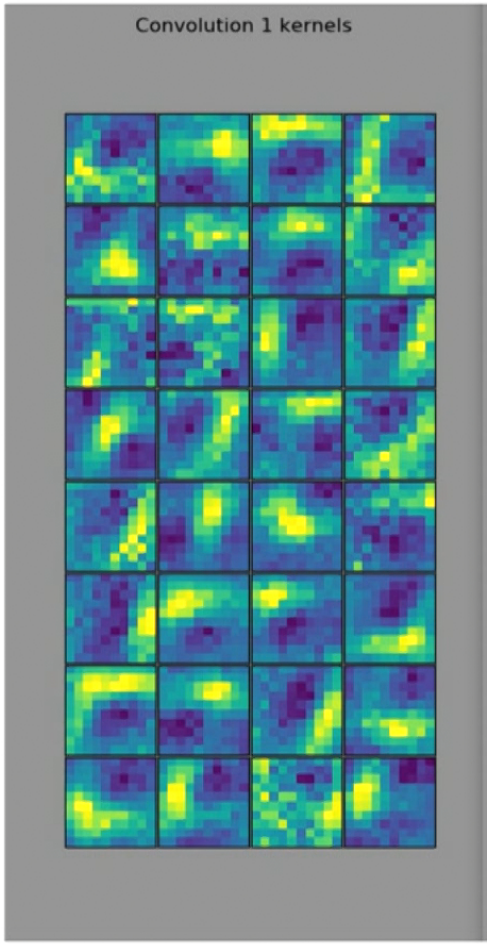
https://www.youtube.com/watch?v=VUkFo6IXMJc

13/23

Feature Extraction







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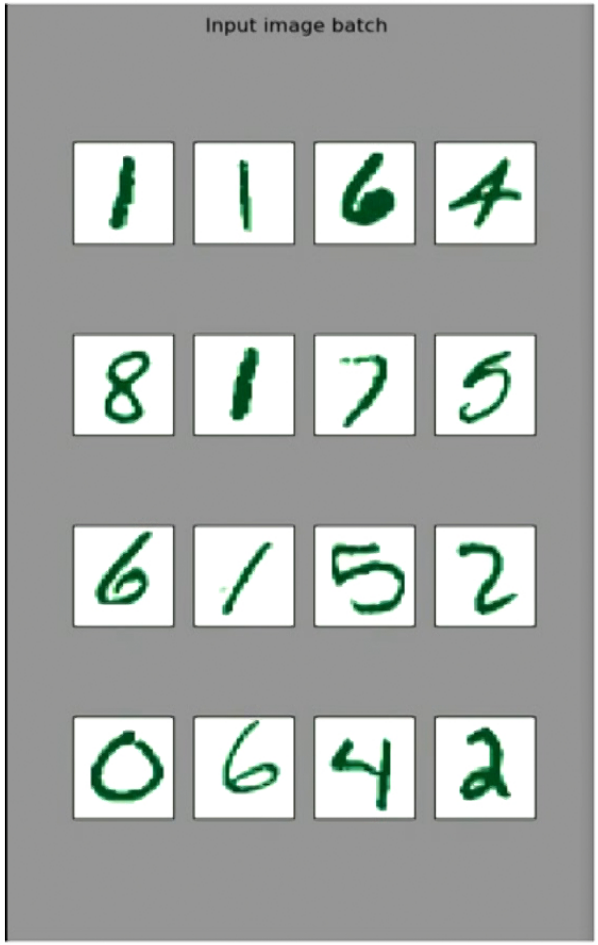

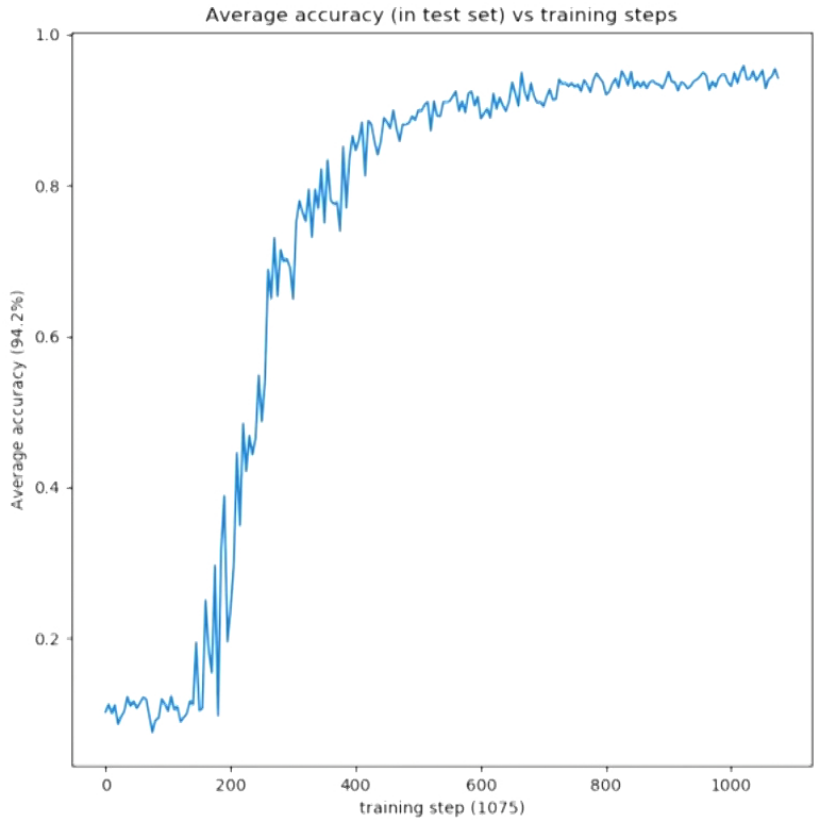

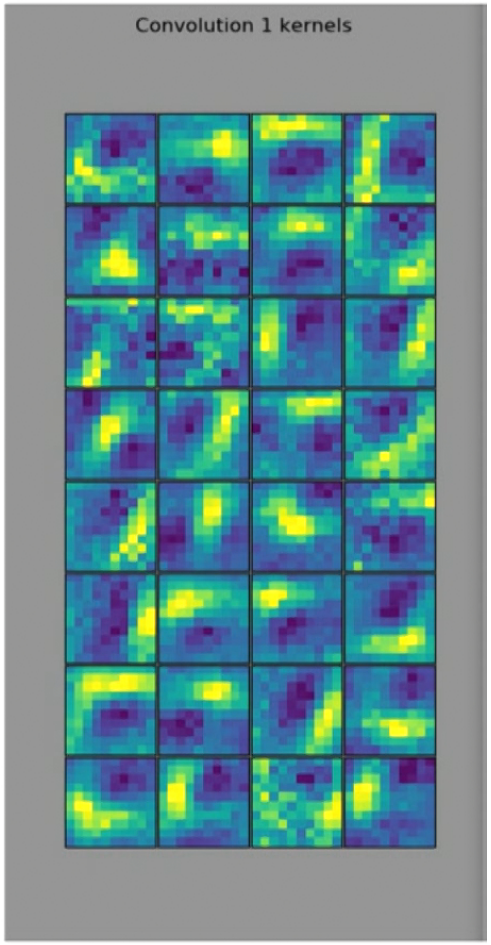

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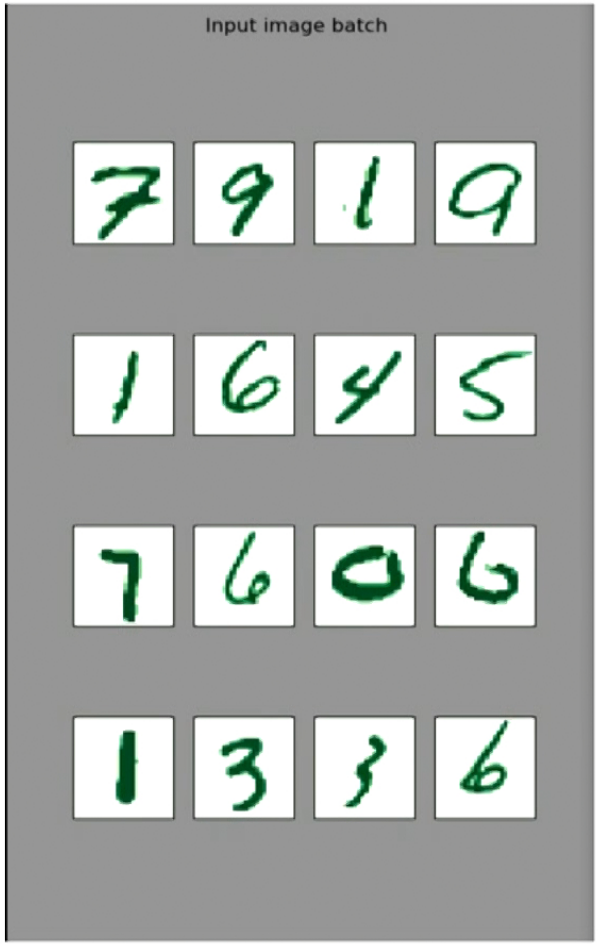

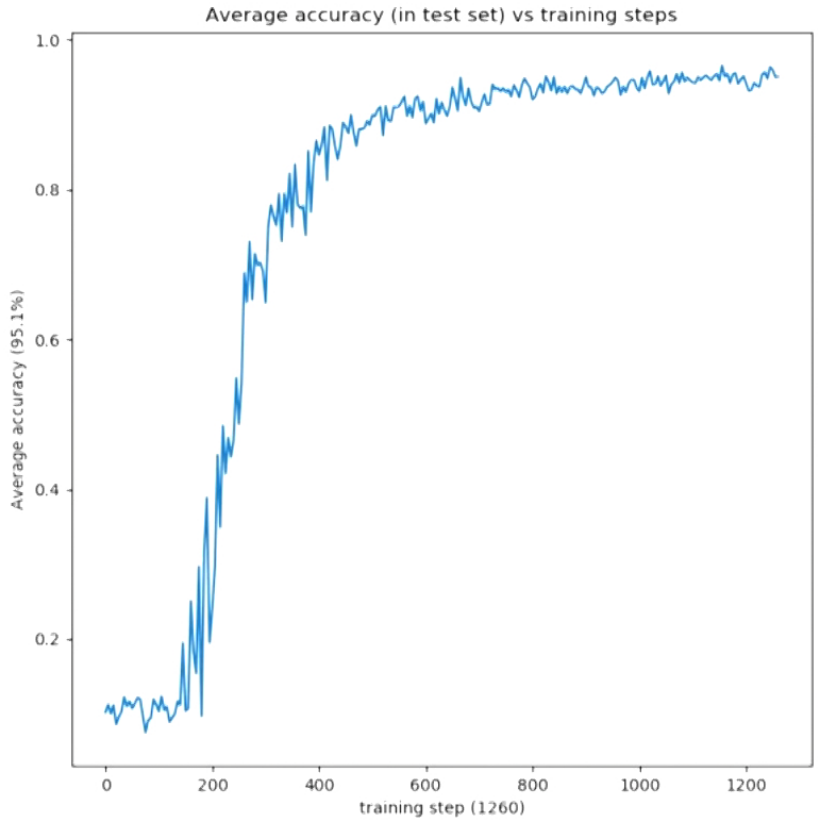

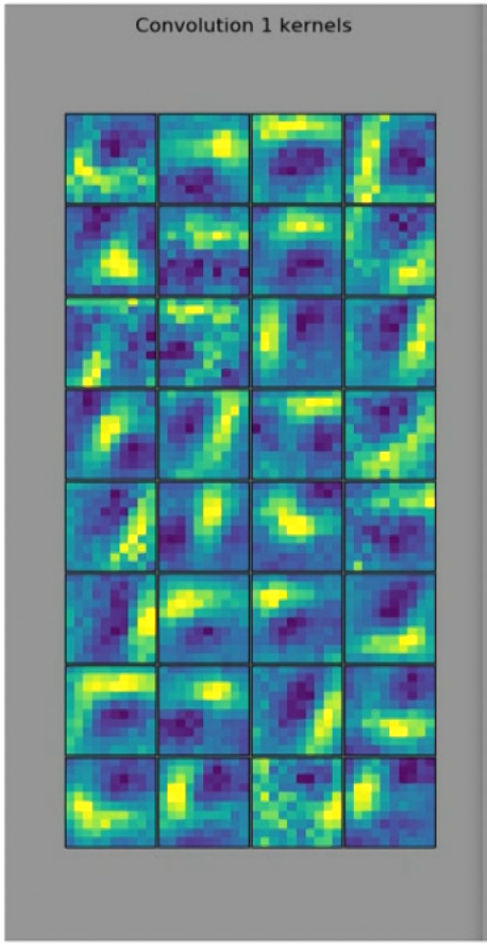

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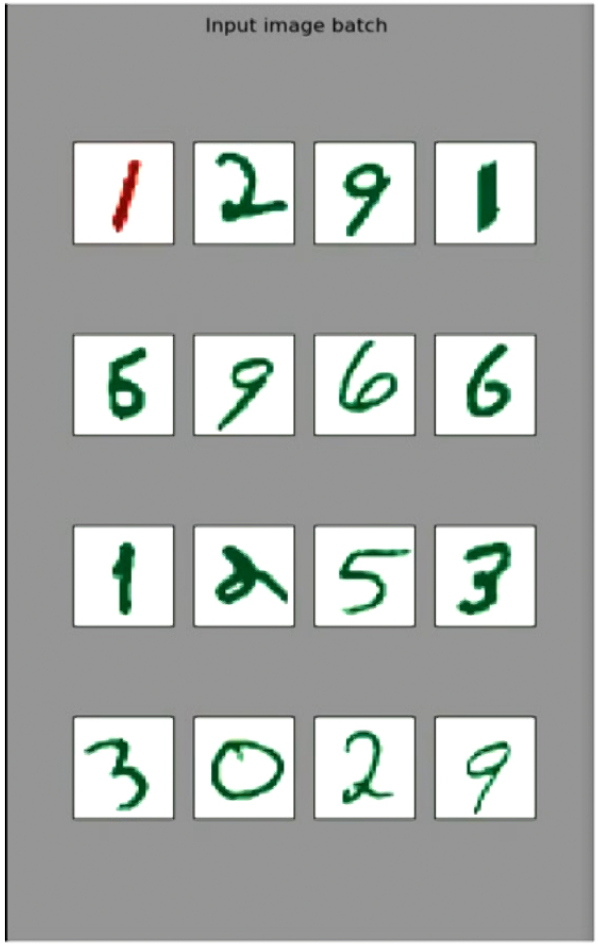

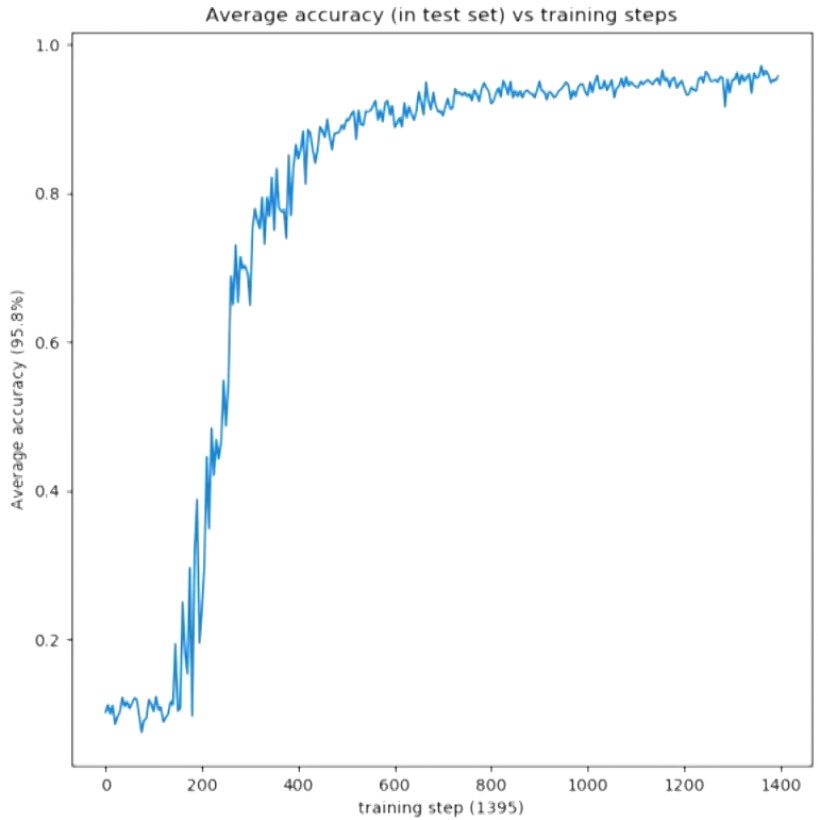

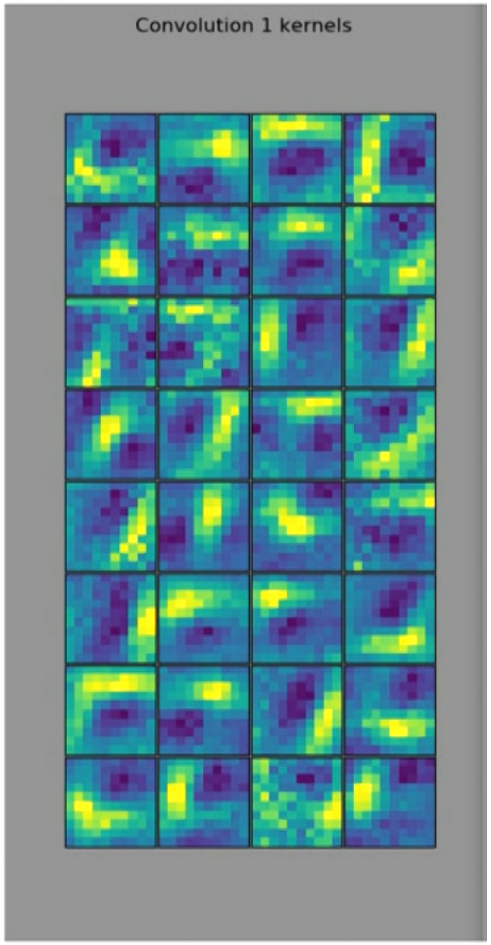

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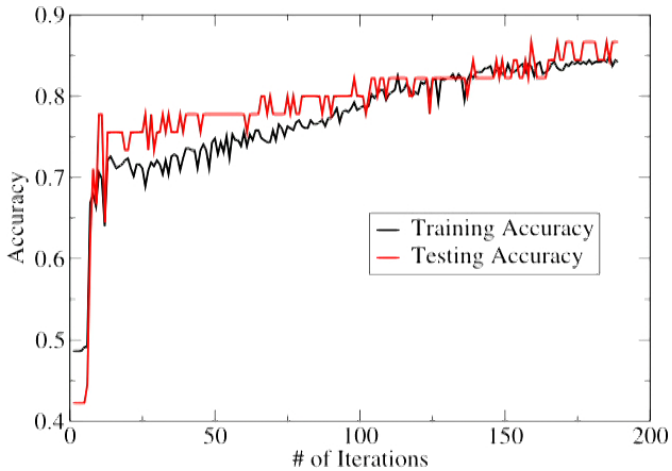
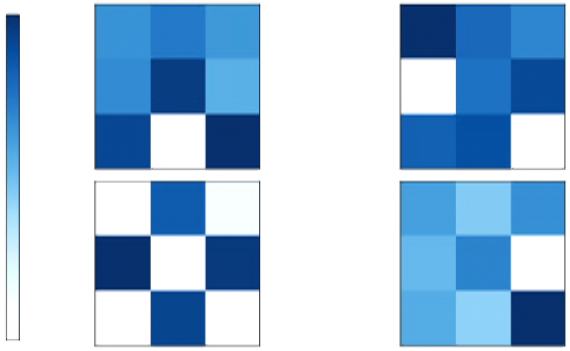
The Many Faces of Non-Fermi Liquid

- **Every panel corresponds to a separate training.**
  - Different trainings have different initial random weights/biases.
- Testing accuracies $\gtrsim$ 86%





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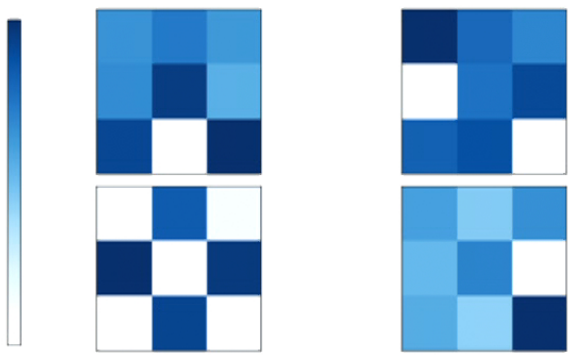

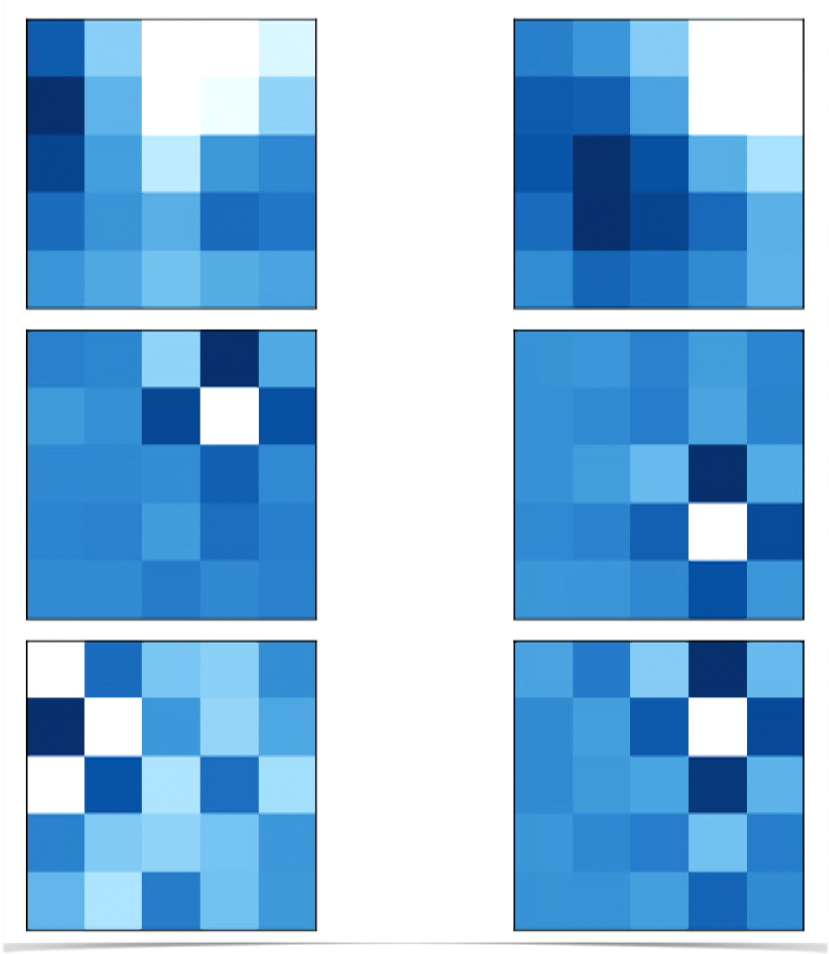

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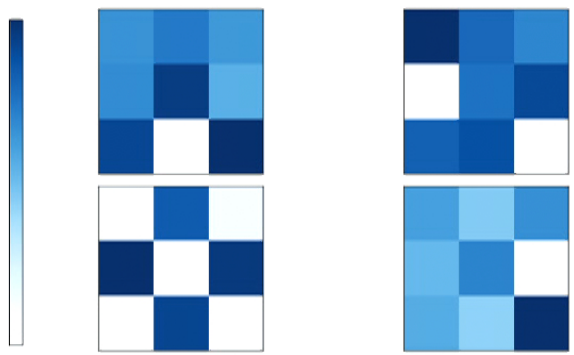
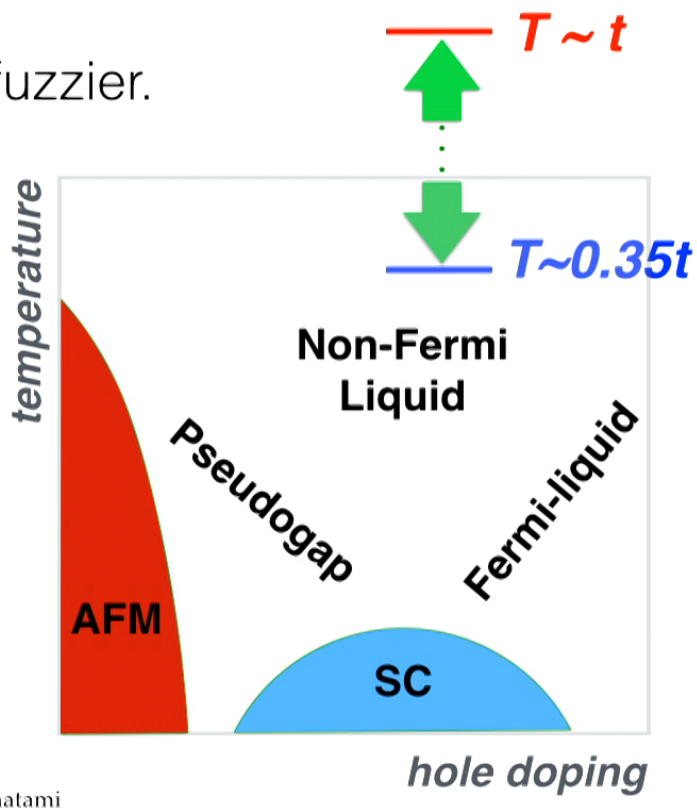
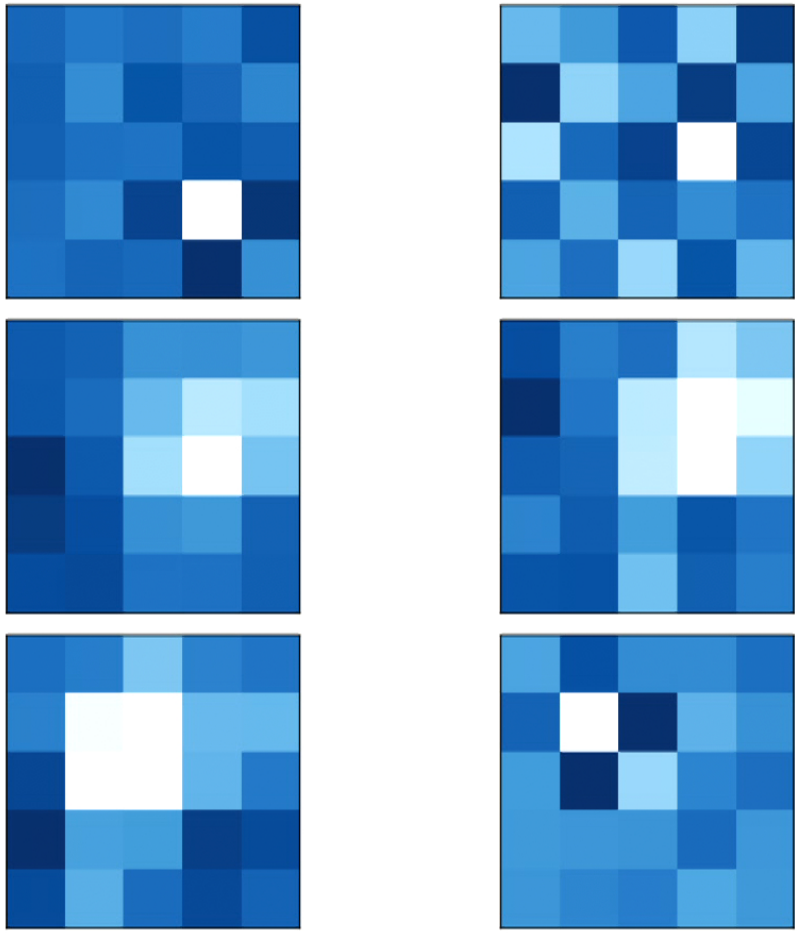


The Many Faces of Non-Fermi Liquid; Closer temperatures

- Features get fuzzier.
- Accuracies decrease to ~70%.



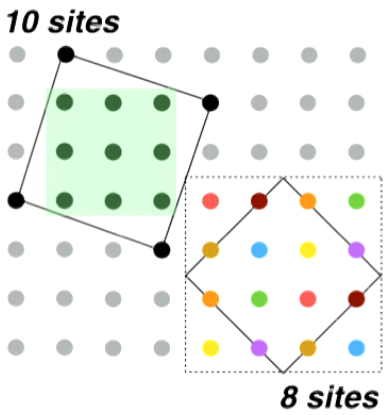


Can We Discover New Physics?

- Can we extract features from the experimental snapshots?
- Do phases like the non-Fermi liquid, pseudogap or d-wave superconductivity have any **signatures in the density basis**?
- Can we use theoretical snapshots to guide future experiment?

Theory Snapshots; ED

Periodic Boundaries



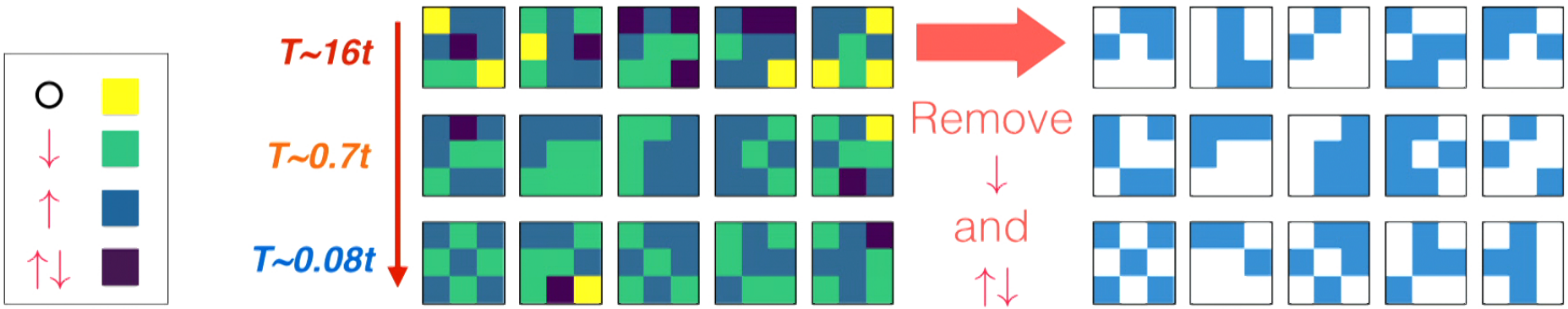
- Solve the Fermi-Hubbard model exactly on small clusters,
- Sample density configurations

$$H = t \sum_{\langle ij \rangle \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

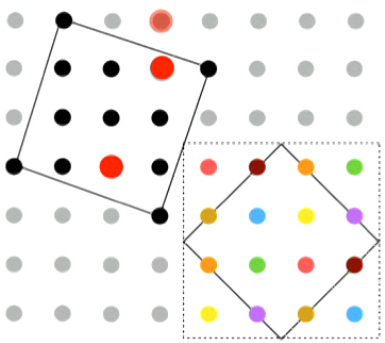
$$U = 8t$$

$$n = 1$$

Pros: Exact; can access any parameter region
Cons: Small sizes (significant boundary effects)



Theory Snapshots; ED



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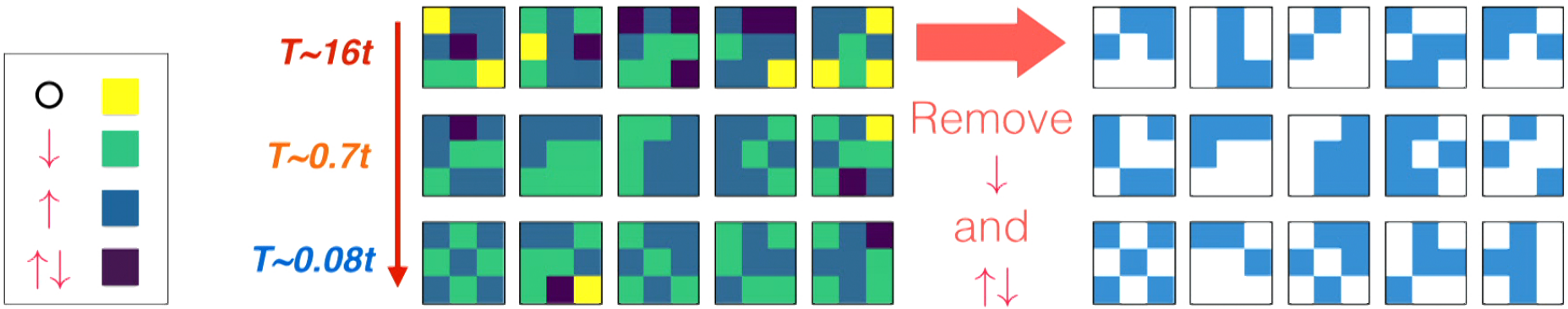
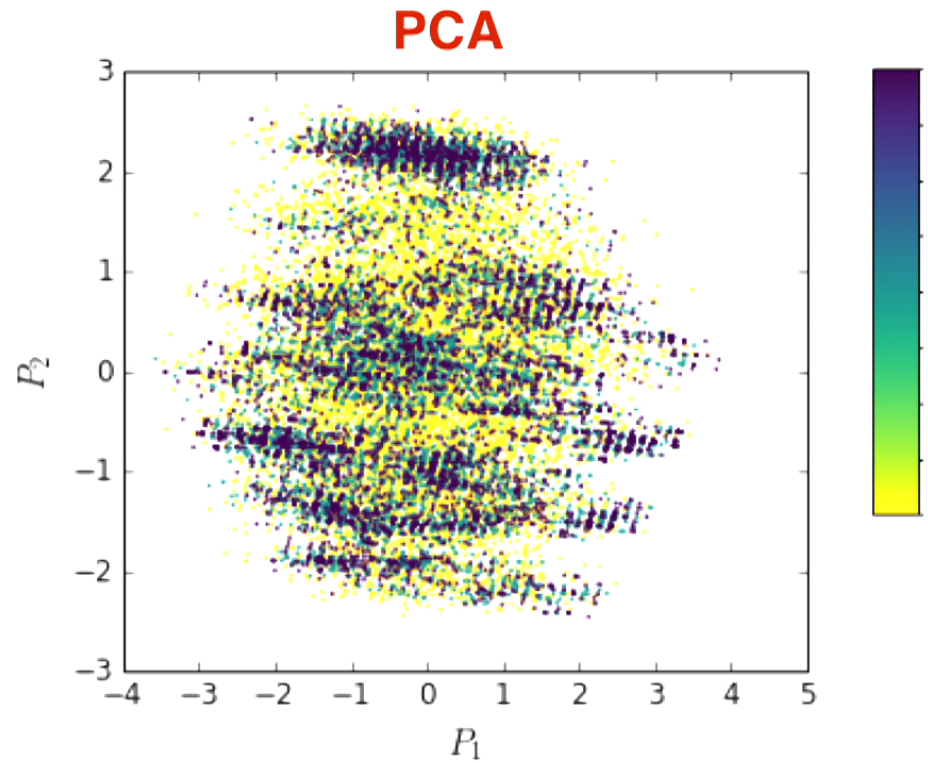
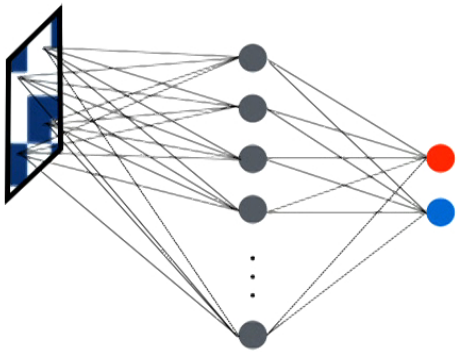


PCA Analysis; ED





	High-T	Mott	AFM
Accuracy	~90%	~78%	Full
	~75%	~68%	Ups (no Doub.)

Theory Snapshots; DQMC

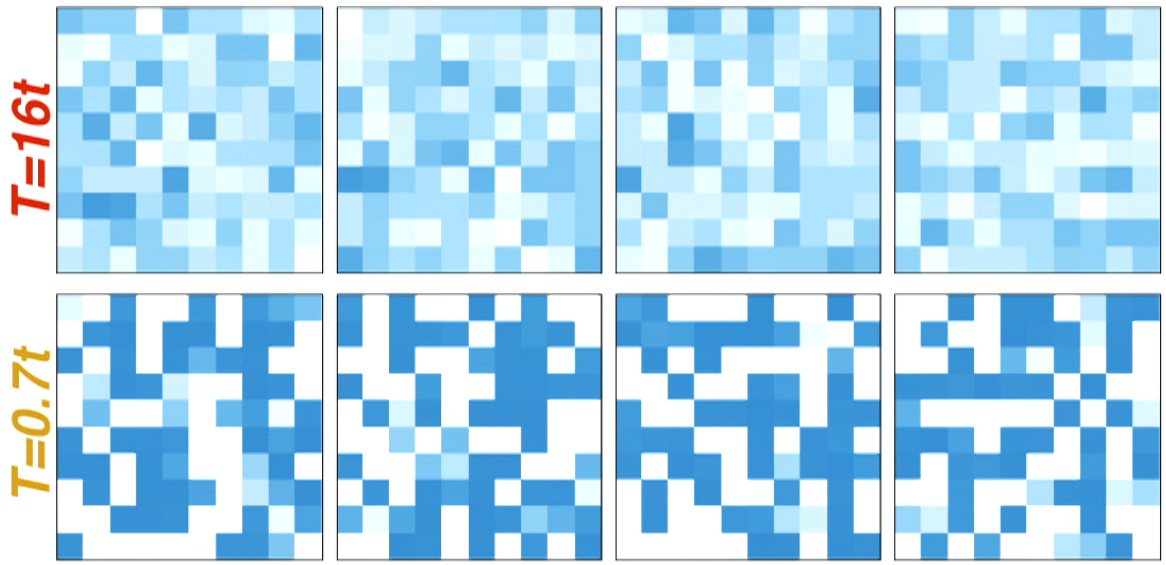
Use Determinant Quantum Monte Carlo to calculate densities for a given auxiliary field configuration during the simulation.

Pros: Can do much larger systems like in the experiments

Cons:

- Not in the particle number basis!
- fuzzy images at hight T,
- sign problem away from half filling (sever below T~0.3t)

*Spin-ups on a **10x10** periodic cluster at **n=0.91***



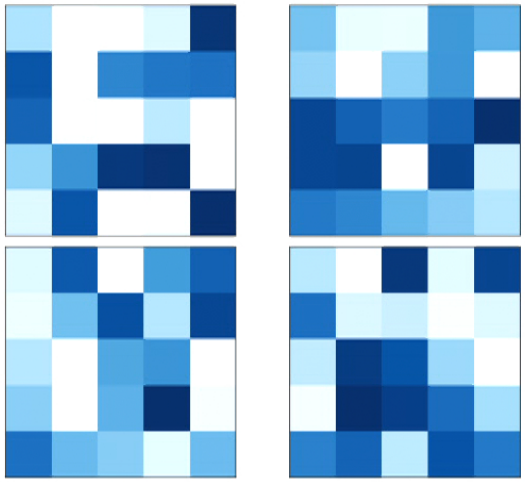
Feature Extraction; DQMC Snapshots

- Similar to features in experimental snapshots, but sharper;

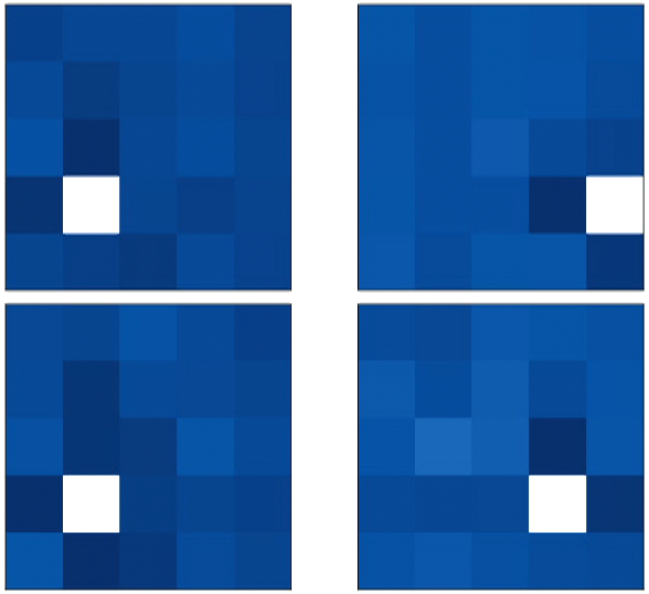
- Similar "random" filters obtained for full-density snapshots

$\boxed{\text{acc.} \gtrsim 96\%}$

Full density



Single species density



Trained with snapshots at the extreme temperature *T=3t* and *T=0.42t* for $U = 8t, n = 0.81$

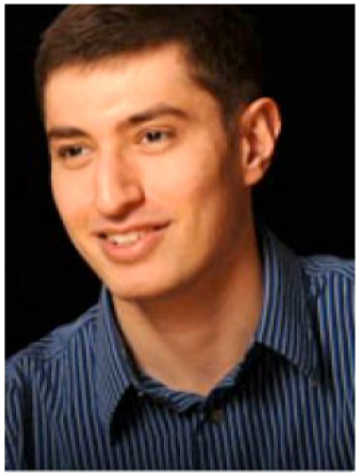
Summary and Outlook

- Filters of trained CNNs show distinct features in the non-Fermi liquid region.
- No discernible patterns emerge with singles density snapshots
- Consistent results are obtained with QMC snapshots.
- Several other improvements can be made
  - Deeper networks (with more data)
  - Augmentation of experimental data
  - Inclusion of the imaginary time dimension for the QMC snapshots

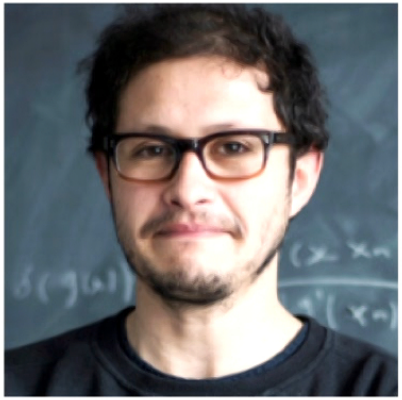
  :

Acknowledgments

Richard Scalettar
(UC Davis)



Waseem Bakr and his group
(Princeton)



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