Title: TBA

Date: Aug 11, 2016 11:00 AM

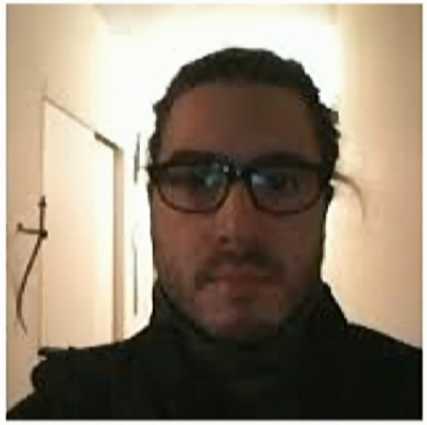
URL: http://pirsa.org/16080015

Abstract:

Collaborators and support

A. von Lilienfeld
Uni Basel

L. F. Arsenault
CU Physics



Richard Neuberg
CU stats

Lauren Hannah
CU Stats & Data Science

Phys. Rev. B90 155136 (2014); arXiv:1506.08858 and to appear

Support: US DOE
Columbia RISE program

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Machine learning

Relation between input (specified by vector of 'descriptors' D) and set of outputs O

$$O(D)=M(D, D_l)$$

Relation determined by intelligent interpolation from outputs O_l produced by learning set D_l

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Many body physics: why bother with machine learning

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Many body physics: why bother with machine learning

- **Solving a many body problem is VERY expensive=>**
  - **Leverage existing results to obtain an inexpensive, approximate solution**

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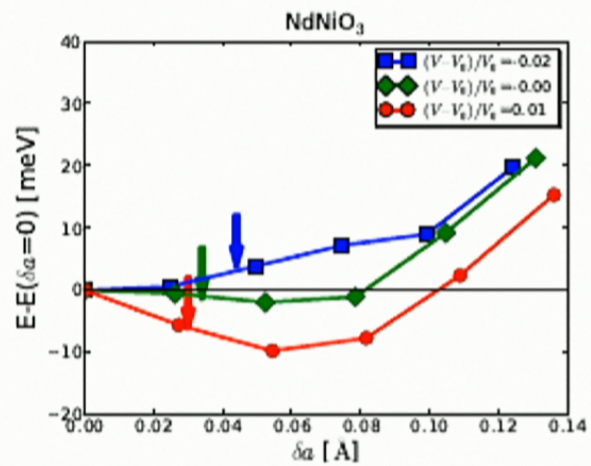
Many body physics: why bother with machine learning

- **Often, need (many) small extrapolations from known solutions**
  - **Structural relaxation (energy as function of many different sets of atomic positions)**
  - **variations in strain and chemical composition**
  - **defect energies and ionic mobilities**



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Many body physics: why bother with machine learning

- State space of quantum many body problems is exponentially big; parameter space of situations to be considered also often very large.

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- `Big data' methods find the relevant very low dimensional subspaces of very high dimensional data sets.

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Many body physics: why bother with machine learning

- State space of quantum many body problems is exponentially big; parameter space of situations to be considered also often very large.
- `Big data' methods find the relevant very low dimensional subspaces of very high dimensional data sets.
- Question (no concrete ideas yet): ?Can these methods give us a way through the wilderness of quantum complexity?

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Machine learning

Questions:

- **What is right set of input descriptors**
- **How do you represent the output**
- **?How big a learning/training set do you need?**

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The Quantum Many Body Problem:

Most common version: electrons in a fixed atomic environment

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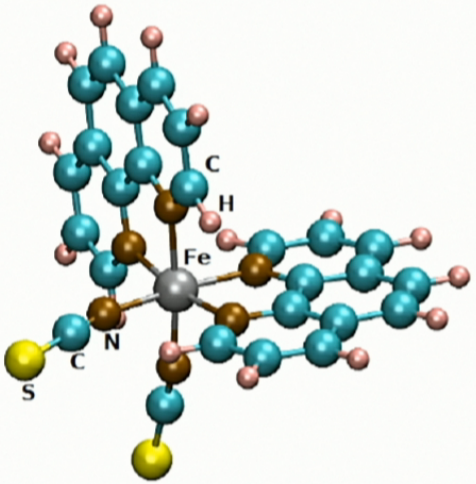
The Quantum Many Body Problem:

Most common version: electrons in a fixed atomic environment

Spin crossover molecule



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The Quantum Many Body Problem:

Most common version: electrons in a fixed atomic environment

Key question: magnetic state of Fe ion

Spin crossover molecule

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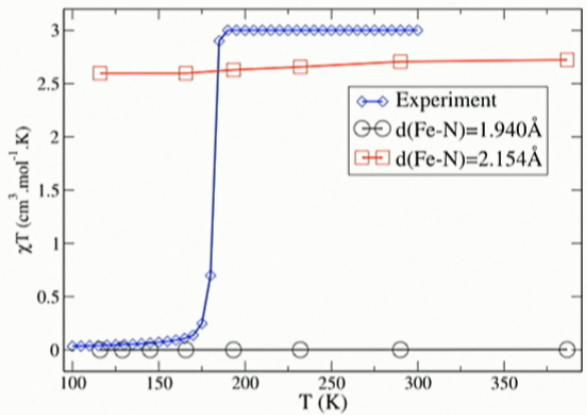
The Quantum Many Body Problem:

Most common version: electrons in a fixed atomic environment

T times magnetic susceptibility vs Temperature



Spin crossover molecule

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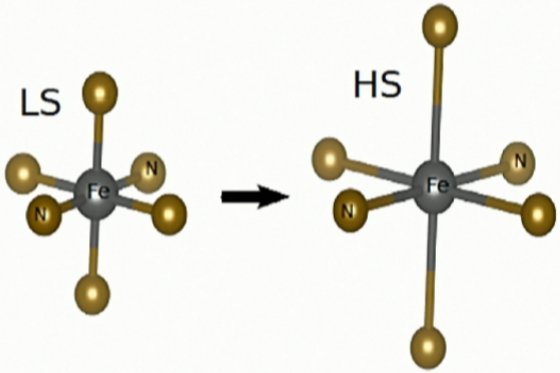
The Quantum Many Body Problem:

Most common version: electrons in a fixed atomic environment

Change of Structure



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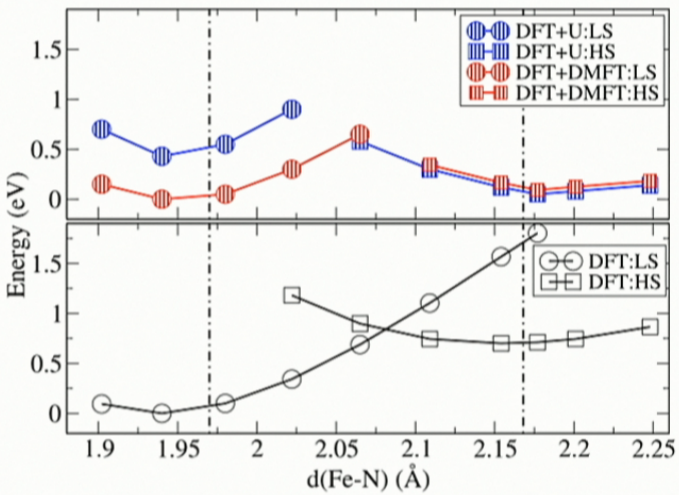
The Quantum Many Body Problem:

Most common version: electrons in a fixed atomic environment

energy vs structure



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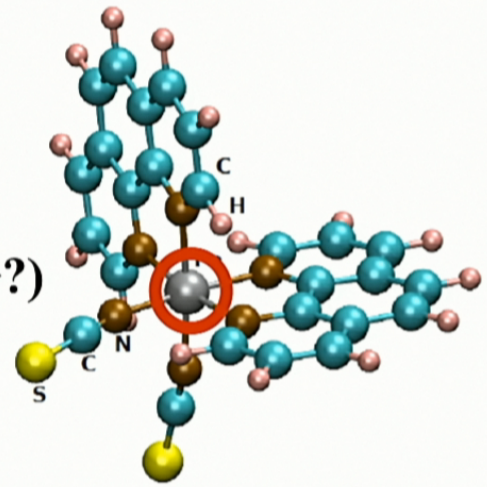

LOTS of (minor) variants:

- Change bond lengths
- Change C-H backbone
- Change immediate Fe environment (N->?)
- Change transition metal ion
- ….

Opportunity for inference from database

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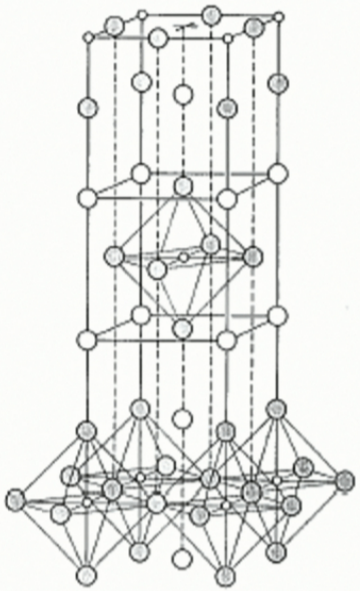
The Quantum Many Body Problem:

High Tc (copper-oxide) superconductivity



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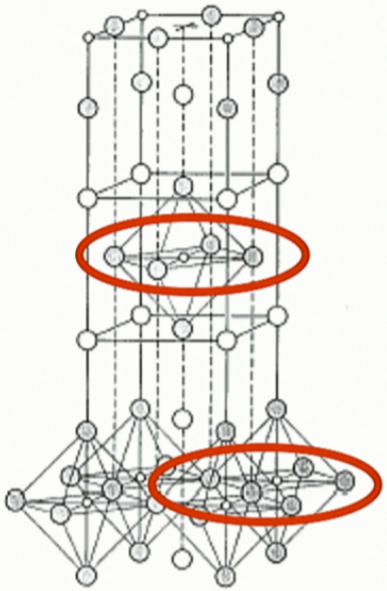
The Quantum Many Body Problem:

High Tc (copper-oxide) superconductivity

Complicated atomic arrangement

- **subset of `relevant' electronic states => minimal theoretical description (``Hubbard model")**



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The Quantum Many Body Problem:

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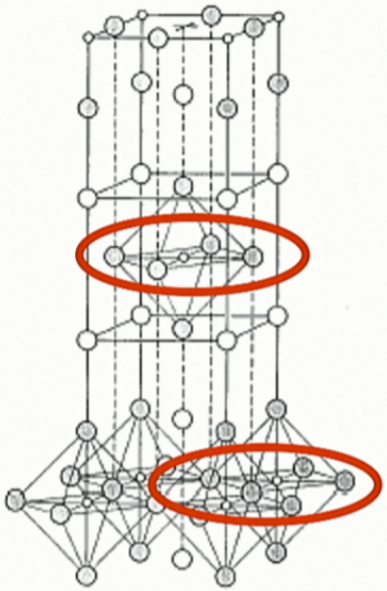

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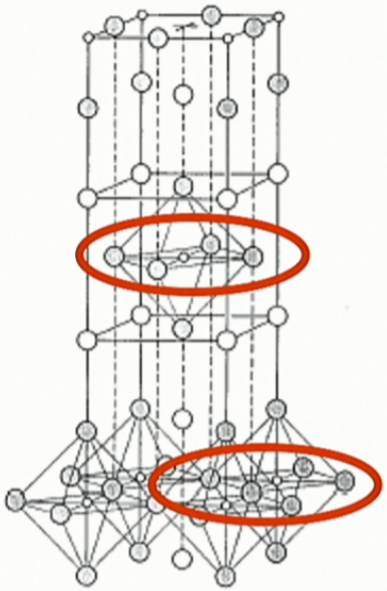
The Quantum Many Body Problem:

High Tc (copper-oxide) superconductivity

Complicated atomic arrangement

- subset of `relevant' electronic states => minimal theoretical description (``Hubbard model")
- many variants (model parameters depend on details of atomic arrangements)
- Question: how do we optimize superconductivity—solve many version of model



Opportunity for inference

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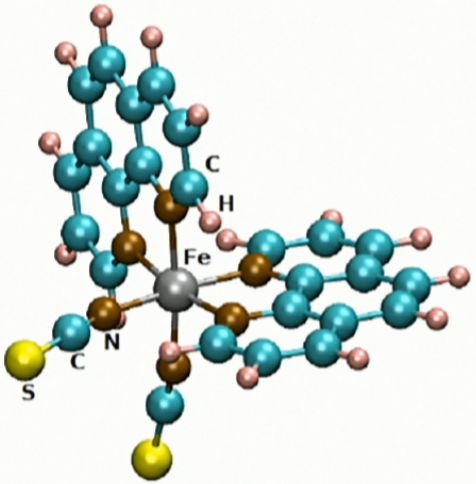
The Quantum Many Body Problem:

The inputs:

``G_0"—electron propagation in reference noninteracting environment: contains information about atomic positions, background electronic structure

``U": electron-electron interaction matrix elements between relevant states



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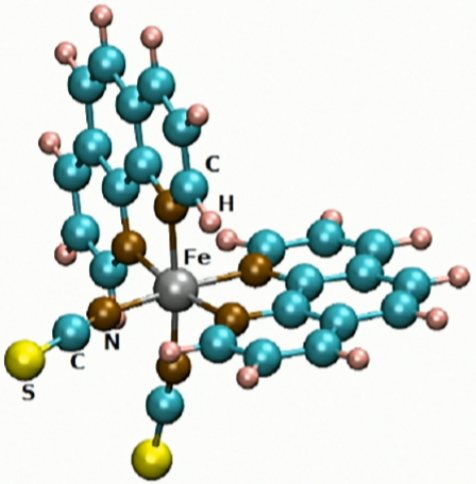
The Quantum Many Body Problem:

The output:

``G"—describes interacting electron behavior in physical system

$''\Sigma''$ —self energy: parametrizes difference in electron behavior between physical system and reference



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The Quantum Many Body Problem: A Functional Relation

Formally: extremizing a functional

$$\Phi[\{G(p,\omega)\}] = \Phi_{univ}[\{G\}] + \mathrm{Trln}\,[G] - \mathrm{Tr}\,[G_0^{-1}G]$$

Interactions ("U") determine Φ_{univ}

Stationarity: $\dfrac{\delta\Phi}{\delta G} = 0$ **determines $G[G_0]$**

=>Need to learn a functional relationship

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=>Need to learn a functional relationship

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Learning functional relations

Need:

- **representation of function (descriptors)**
- **way to impose constraints**

Would like to know

- **Size of needed database**
- **Accuracy of prediction:**
  - **global fit**
  - **particular physically relevant aspects**
- **Back-inference—can we design desired behavior**

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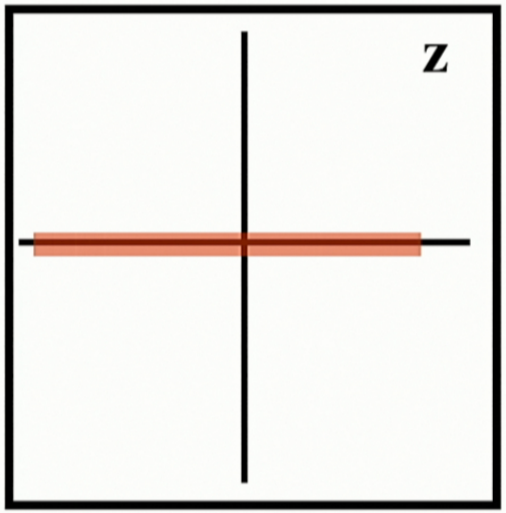
A mathematical digression

G(z) is analytic in complex frequency (z) plane

except for branch cut discontinuity across Im z=0



Spectral function:

$$\mathbf{A}(\omega) = \frac{\mathbf{G}(\omega - \mathbf{i}\delta) - \mathbf{G}(\omega + \mathbf{i}\delta)}{\mathbf{2i}}$$

is non-negative, integrates to Pi, and (typically) has compact support

has physical meaning of density of states: prob to add or remove particle

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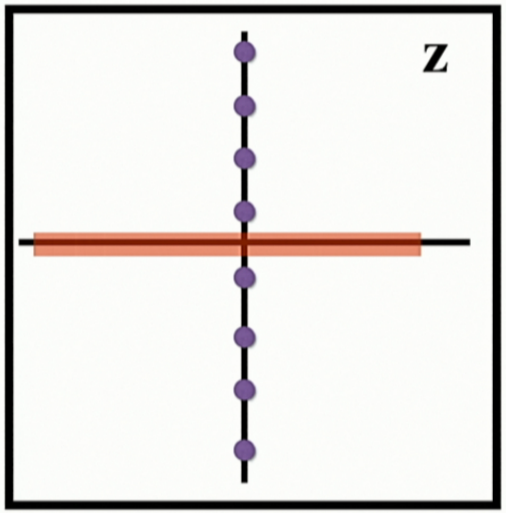
$$\Rightarrow \boxed{G(z) = \int \frac{dx}{\pi} \frac{A(x)}{z - x}}$$



Convenient to evaluate G on imaginary frequency axis at points

$$z_n = i\omega_n \equiv (2n+1)\pi T$$

or to construct

$$G(\tau) = T \sum_n e^{i\omega_n \tau} G(i\omega_n)$$

Complex variable theory: A can be reconstructed from $G(z_n)$

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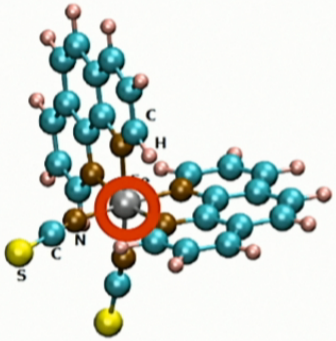
Learning Many Body Physics: Step 1: the Anderson Model

One (spin-degenerate) interacting level coupled to a bath of noninteracting electrons



$$H = \sum_{\sigma} \varepsilon_d d_\sigma^\dagger d_\sigma + U d_\uparrow^\dagger d_\uparrow d_\downarrow^\dagger d_\downarrow$$

$$+ \sum_{k,\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_{k,\sigma} V_k \left(d_\sigma^\dagger c_{k\sigma} + c_{k\sigma}^\dagger d_\sigma \right).$$

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The Anderson Model

One (spin-degenerate) interacting level coupled to a bath of noninteracting electrons

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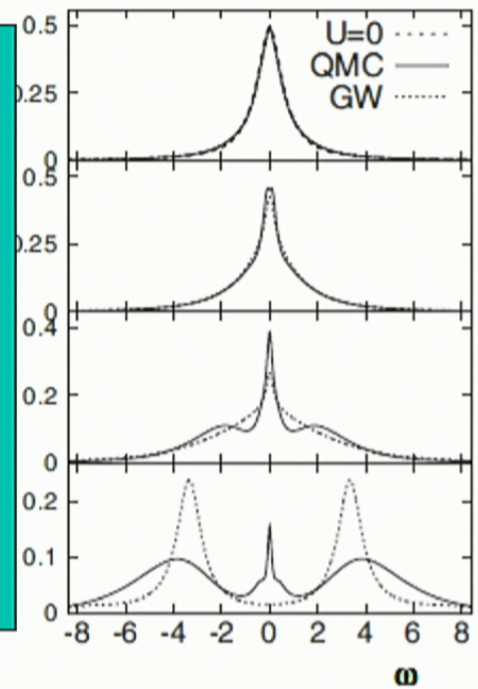
Many-body density of states

$$A(\omega) = \mathrm{Im}G(\omega - i\delta)$$



U increases ->

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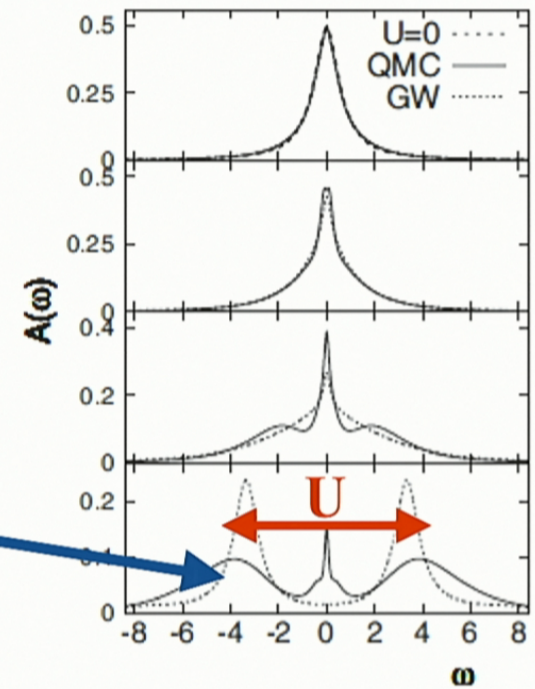

U increases ->

Side-bands

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The Anderson Model

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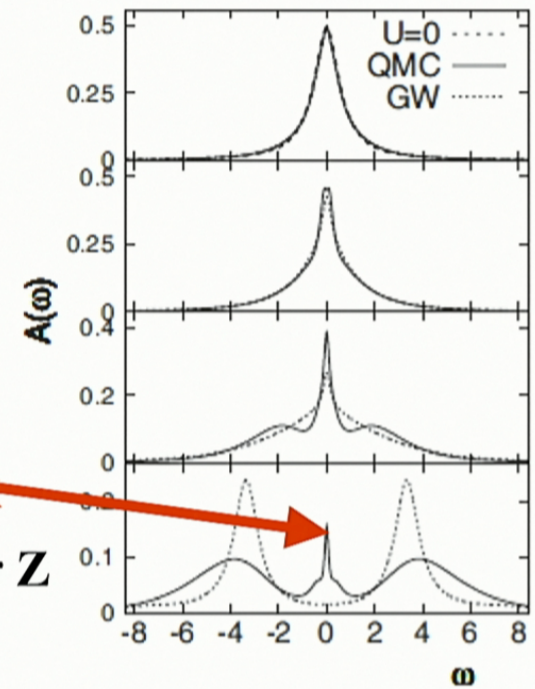
Many-body density of states



Central (Kondo) peak

Width=>renormalization factor Z

U increases ->

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Anderson Model: Inputs

One (spin-degenerate) interacting level coupled to a bath of noninteracting electrons

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Bath characterized by

$$\mathbf{N}(\omega) = \pi \sum_k V_k^2 \delta(\omega - \varepsilon_k)$$

Details not important. We choose

$$\mathbf{N}(\omega) = V^2 \sqrt{1 - \omega^2} \quad (\omega^2 < 1)$$

=>parameter is V

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The Anderson Model: Inputs

One (spin-degenerate) interacting level coupled to a bath of noninteracting electrons

<=> occupancy of d-level, n_d

$$H = \sum_{\sigma} \varepsilon_d d_\sigma^\dagger d_\sigma + U d_\uparrow^\dagger d_\uparrow d_\downarrow^\dagger d_\downarrow$$

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Interaction

descriptor:

(V, U, n_d)

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The Anderson Model: Output

One (spin-degenerate) interacting level coupled to a bath of noninteracting electrons

$$\mathbf{G}(\tau) = -\left\langle \mathbf{d}_\sigma(\tau)\mathbf{d}_\sigma^\dagger(\mathbf{0})\right\rangle$$

$$H = \sum_\sigma \varepsilon_d d_\sigma^\dagger d_\sigma + U d_\uparrow^\dagger d_\uparrow d_\downarrow^\dagger d_\downarrow$$

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Represented as:

- **Coefficients of Legendre polynomials**
- **Continued fraction expansion**
- **Values at frequencies z_n**

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The Anderson Model: method

One (spin-degenerate) interacting level coupled to a bath of noninteracting electrons

$$H = \sum_{\sigma} \varepsilon_d d_\sigma^\dagger d_\sigma + U d_\uparrow^\dagger d_\uparrow d_\downarrow^\dagger d_\downarrow$$
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Kernel Ridge Regression

$$g_m(\mathbf{D}) = \sum_l \alpha_{lm} K_m(\mathbf{D}_l, \mathbf{D})$$

Kernel

$$K(\mathbf{D}_i, \mathbf{D}) = \mathrm{e}^{-\frac{|\boldsymbol{d}_i|}{\sigma}}$$

- **Simple exponential kernel worked best.**
- **d =Manhattan distance. Width large (~10)**

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The Anderson Model: method

One (spin-degenerate) interacting level coupled to a bath of noninteracting electrons

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Kernel Ridge Regression

$$g_m(\mathbf{D}) = \sum_l \alpha_{lm} K_m(\mathbf{D}_l, \mathbf{D})$$

coefficients fixed by training set

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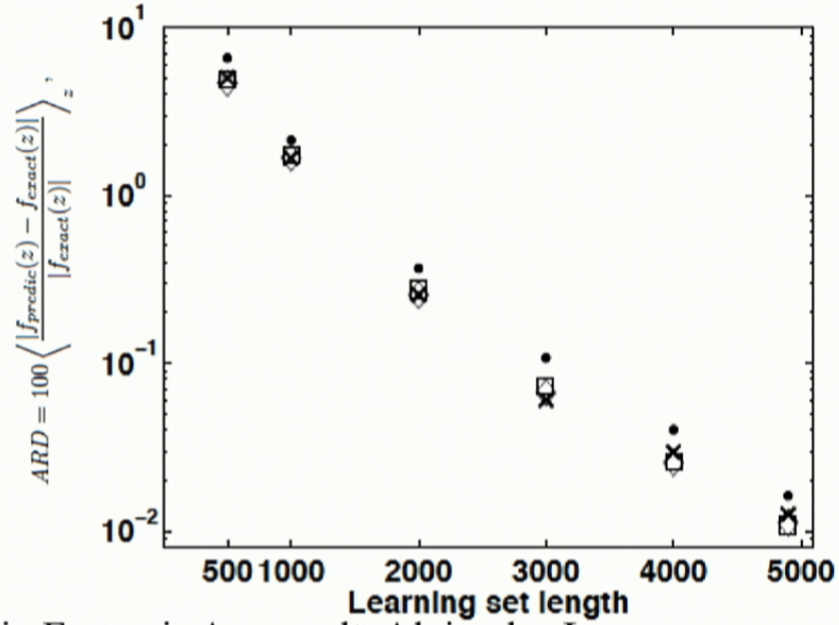
The Anderson Model: Results

Error averaged over some low order coefficients as function of learning set length



● Continued fraction

x z_n

□ Time

◇ Legendre

Learning set size ~1000 needed

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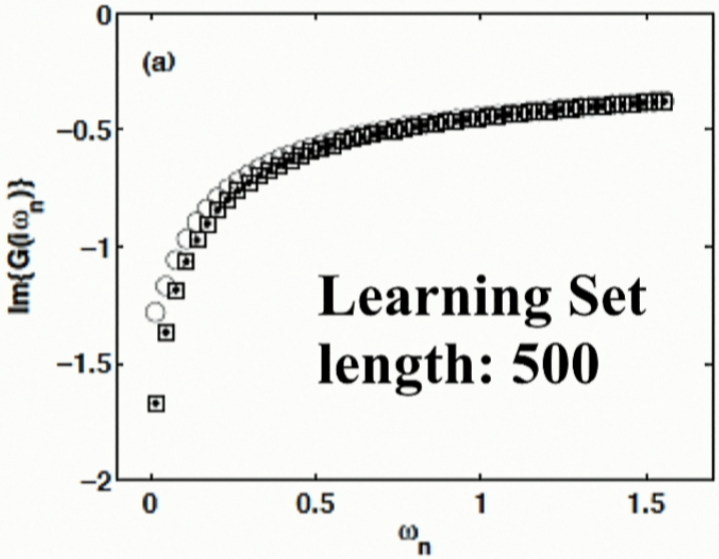
The Anderson Model: Results

Learning Features of G and A: continued fraction representation



- **Exact**
- **ML result**

Louis-Francois Arsenault, Alejandro Lopez-Bezanilla, O. Anatole von Lilienfeld, A. J.M., Phys. Rev. B90 155136 (2014).

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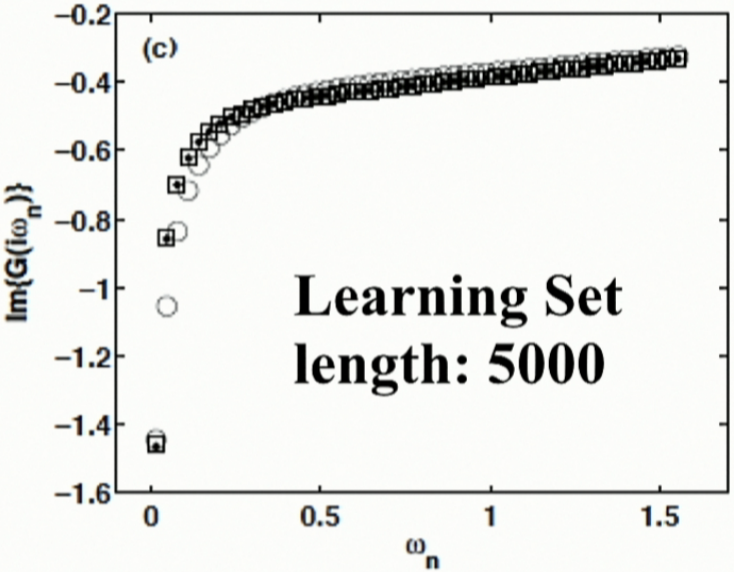

- ● Exact
- ○ ML result

Learning set size ~1000 needed

Louis-Francois Arsenault, Alejandro Lopez-Bezanilla, O. Anatole von Lilienfeld, A. J.M., Phys. Rev. B90 155136 (2014).

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The Anderson Model: Results

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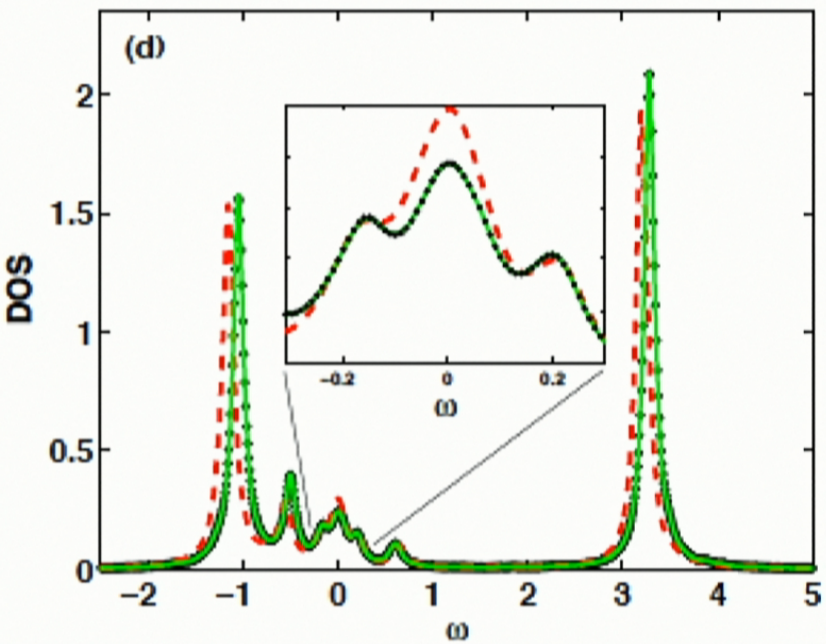

- Exact
- ML: 500
- ML: 5000

Bezanilla, O. Anatole von Lilienfeld, A. J.M., Phys. Rev. B90 155136 (2014).

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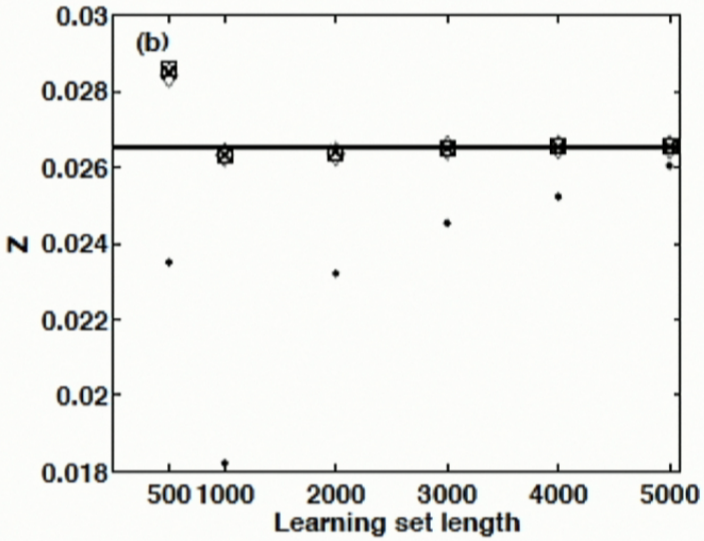
The Anderson Model: Results

the quasiparticle weight Z



- ● **Continued fraction**
- X **z_n**
- □ **Time**
- ◇ **Legendre**

Learning set size >1000 needed

Legendre rep. preferred because most compact

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The Anderson Model: Results

- We can learn functions
- Legendre rep. preferred (most compact representation; minimizes dimension of input space)
- Required dataset is not small

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Learning a lattice many-body problem

$$\mathbf{H} = \sum_{\mathbf{ij}\sigma} \mathbf{t_{ij}} \mathbf{c}^{\dagger}_{\mathbf{i}\sigma} \mathbf{c}_{\mathbf{j}\sigma} + \mathbf{U} \sum_{\mathbf{i}} \hat{\mathbf{n}}_{\mathbf{i}\uparrow} \hat{\mathbf{n}}_{\mathbf{i}\downarrow}$$

Model has two phases:

- **Mott Insulator: n=1, large U. Characterized by gap**
- **Metal, n\neq 1 or U not large. Characterized by mass enhancement**

We will learn a particular approximate solution, obtained by the `dynamical mean field' method

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Learning a lattice many-body problem

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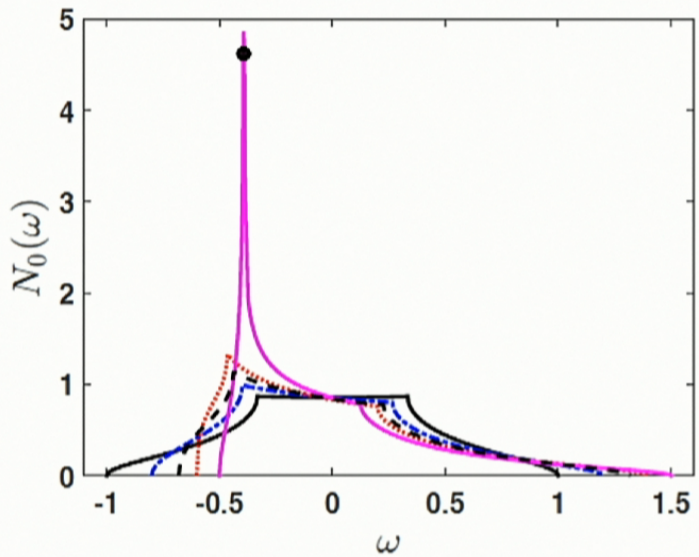
Descriptors:

- density of states (t_{ij}): Legendre coeffs
- U
- electron density

Output:

- phase (metal or insulator)
- G (Legendre coeffs)



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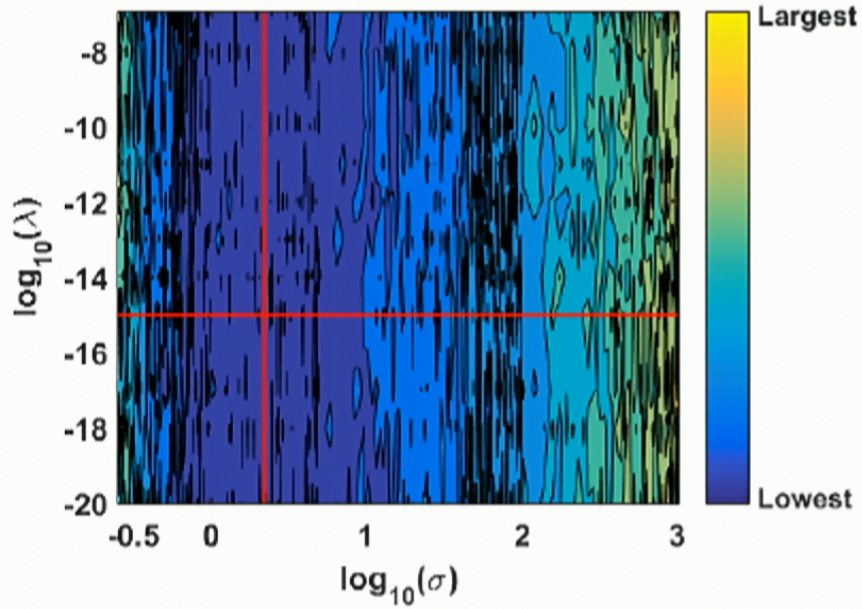
Learning a lattice many-body problem

$$\mathbf{H} = \sum_{\mathbf{ij}\sigma} \mathbf{t_{ij}} \mathbf{c}^{\dagger}_{\mathbf{i}\sigma} \mathbf{c}_{\mathbf{j}\sigma} + \mathbf{U} \sum_{\mathbf{i}} \hat{\mathbf{n}}_{\mathbf{i}\uparrow} \hat{\mathbf{n}}_{\mathbf{i}\downarrow}$$

Technical improvement: cross validation

Pick ML hyperparameters to minimize error in 1st 5 Legendre coeffs of 1000 examples



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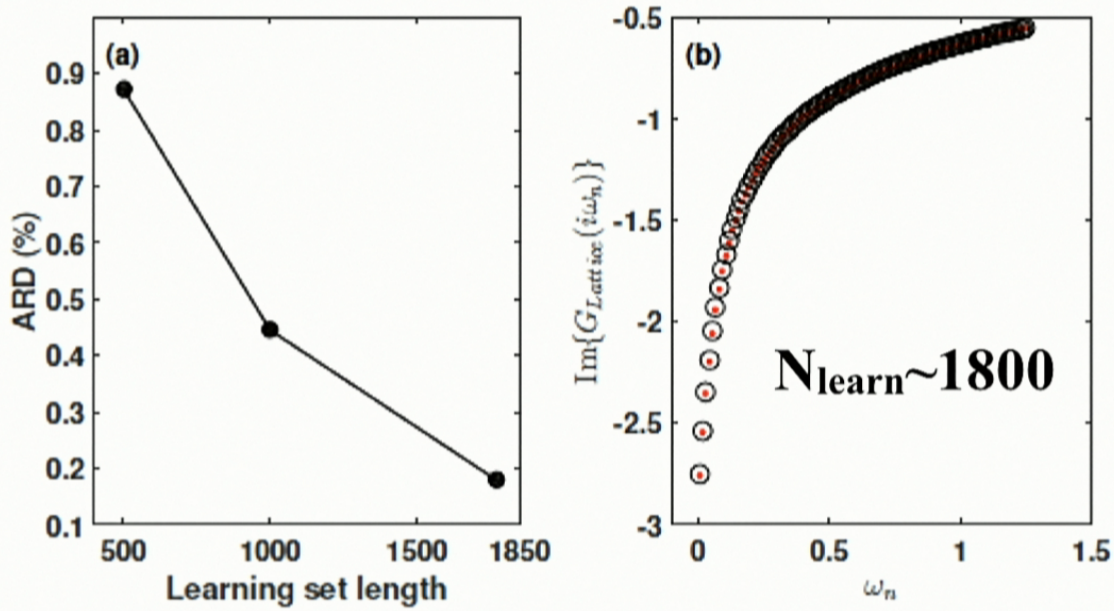
Cross-validation leads to much smaller errors



Training sets of ~few hundred are acceptable

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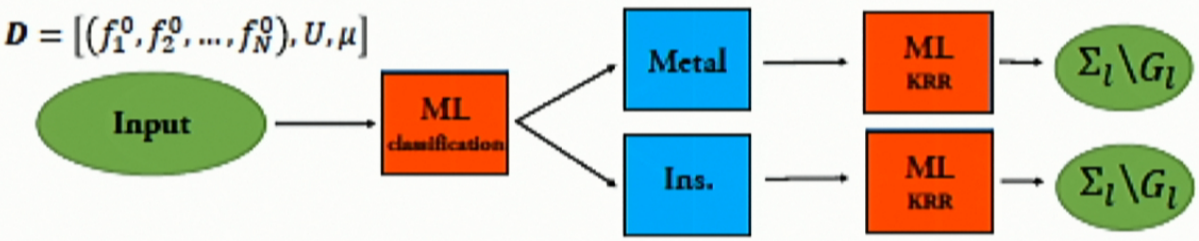
Learning a lattice many-body problem

$$\mathbf{H} = \sum_{\mathbf{ij}\sigma} \mathbf{t_{ij}} \mathbf{c}^{\dagger}_{\mathbf{i}\sigma} \mathbf{c}_{\mathbf{j}\sigma} + \mathbf{U} \sum_{\mathbf{i}} \hat{\mathbf{n}}_{\mathbf{i}\uparrow} \hat{\mathbf{n}}_{\mathbf{i}\downarrow}$$

2 step learning:

- **Classification**
- **Greens function (self energy)**



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Classification

- **Random Decision Forest**
- **Use 1st 5 Legendre coeffs of DOS plus U,mu**

Classification: Almost perfectly accurate

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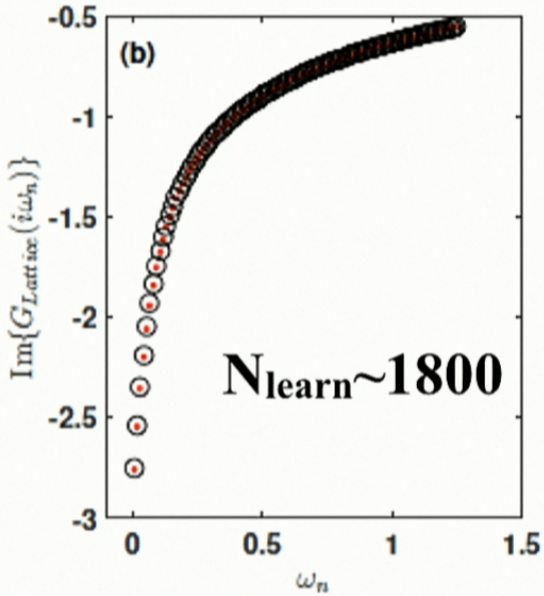
Learning a lattice many-body problem

$$\mathbf{H} = \sum_{\mathbf{ij}\sigma} \mathbf{t_{ij}} \mathbf{c}^{\dagger}_{\mathbf{i}\sigma} \mathbf{c}_{\mathbf{j}\sigma} + \mathbf{U} \sum_{\mathbf{i}} \hat{\mathbf{n}}_{\mathbf{i}\uparrow} \hat{\mathbf{n}}_{\mathbf{i}\downarrow}$$



G reproduced perfectly

- **Exact**
- **ML**

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reverse engineering a lattice many-body problem

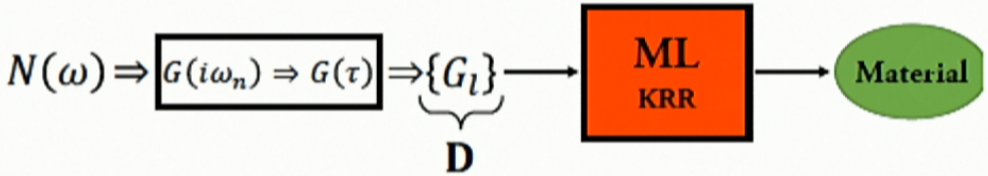
$$\mathbf{H} = \sum_{\mathbf{ij}\sigma} \mathbf{t_{ij}} \mathbf{c}^{\dagger}_{\mathbf{i}\sigma} \mathbf{c}_{\mathbf{j}\sigma} + \mathbf{U} \sum_{\mathbf{i}} \hat{\mathbf{n}}_{\mathbf{i}\uparrow} \hat{\mathbf{n}}_{\mathbf{i}\downarrow}$$

Question:

What t_{ij} should I use to get a desired many-body DOS?

Answer:

Run the `machine' backwards



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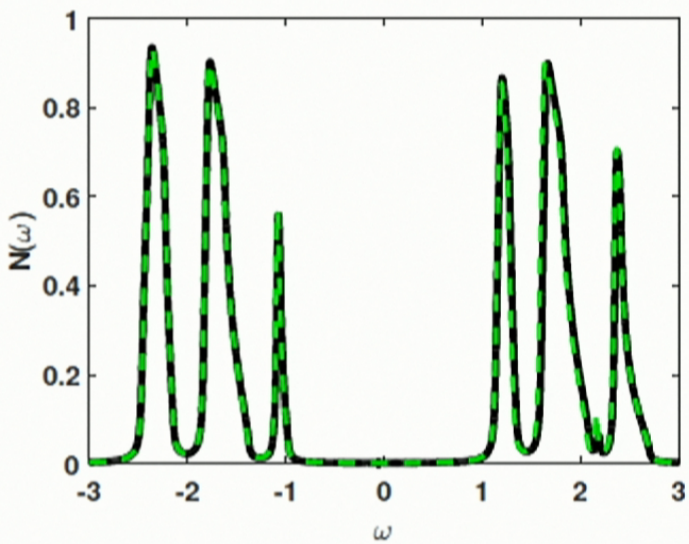
reverse engineering a lattice many-body problem

$$N(\omega) \Rightarrow \boxed{G(i\omega_n) \Rightarrow G(\tau)} \Rightarrow \underbrace{\{G_l\}}_{\mathbf{D}} \longrightarrow \boxed{\begin{matrix}\text{ML}\\ \text{KRR}\end{matrix}} \longrightarrow \text{Material}$$



Target: gap of size 2. Method works with database of ~200 examples

Result

Target

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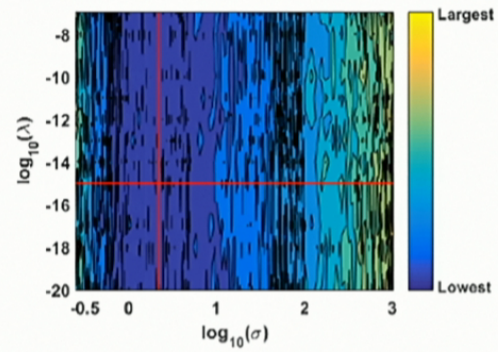
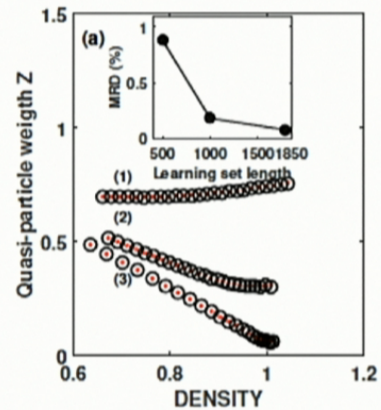
Summary

- Cross-validation + intelligent representation of functions =>
- many-body problems can be learned+reverse engineering done
- Needed training data sets not outrageously big
- Key point: represent input and output functions in compact orthogonal function basis





?Extension to realistic situation?

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Coda: analytical continuation

$$\boxed{G(z) = \int \frac{dx}{\pi} \frac{A(x)}{z - x}}$$

Math: if you know G on the points (all n)

$$z_n = i\omega_n \equiv (2n+1)\pi T$$

you can reconstruct A.

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The difficulty:

The operator

$$K(z, x) = \frac{1}{z - x}$$

has many very small eigenvalues.
=> inversion is ill-posed.
Small errors in $G(z_n)$ lead to big errors in inferred A

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$$z_n = i\omega_n \equiv (2n+1)\pi T$$

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the standard solution: maximum entropy

Minimize

$$\mathbf{F} = \sum_{\mathbf{n}} |\mathbf{G}(\mathbf{z_n}) - \mathbf{K}(\mathbf{z_n}, \mathbf{x}) * \mathbf{A}(\mathbf{x})|^2 + \alpha \int \mathbf{dx}\ \mathbf{A}(\mathbf{x}) \ln \frac{\mathbf{A}(\mathbf{x})}{\mathbf{M}(\mathbf{x})}$$

with respect to A(x).

***Need `model function' M(x) and parameter alpha**
***No method for assessing errors.**

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Instead: 'learn' the solution

=>

view problem as statistical inference, not as operator inversion

- Forward problem (G given A) is computationally trivial=>easy to get large database
- Regression =>regularization: eliminates very small eigenvalues (at the expense of removing sharp features from result)
- constraints (positivity, unit area) imposed by projection
- **Error estimates available**

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Technical point: representation of functions

Represent A by conformal coefficients

$$\mathbf{A}(\omega) = \sum_{\mathbf{n}=-\infty}^{\infty} \mathbf{a_n} \left(\frac{\omega - \mathbf{i}\omega_0}{\omega + \mathbf{i}\omega_0} \right)^{\mathbf{n}}$$

$$\mathbf{a}_n = \oint \frac{dz}{2\pi i} \frac{A\left(i\omega_0 \left(\frac{1+z}{1-z}\right)\right)}{z^{n+1}}$$

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Learning and Tuning Sets

Many examples, constructed as sums of Gaussians

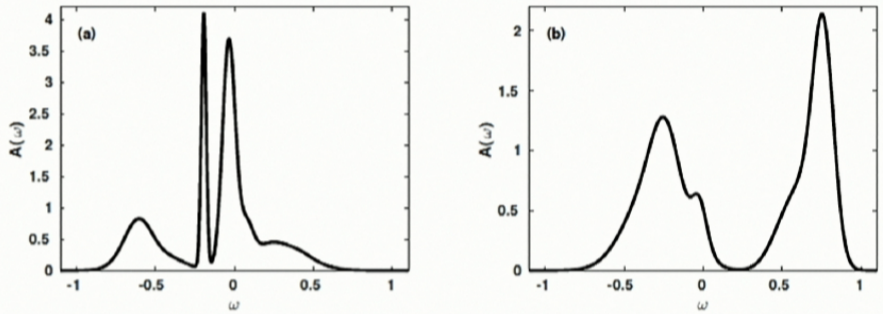
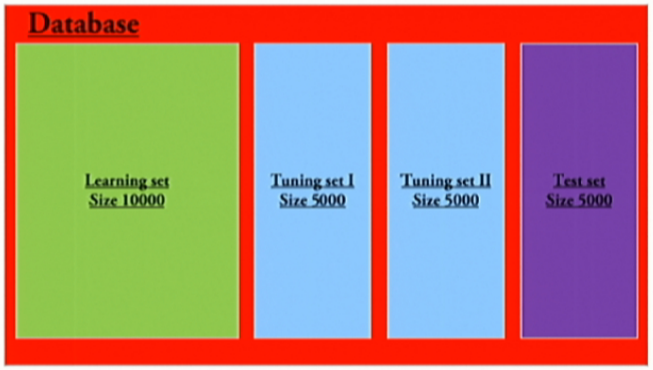


Figure 1: Two different (a) and (b) possible $A(\omega)$ in the database.



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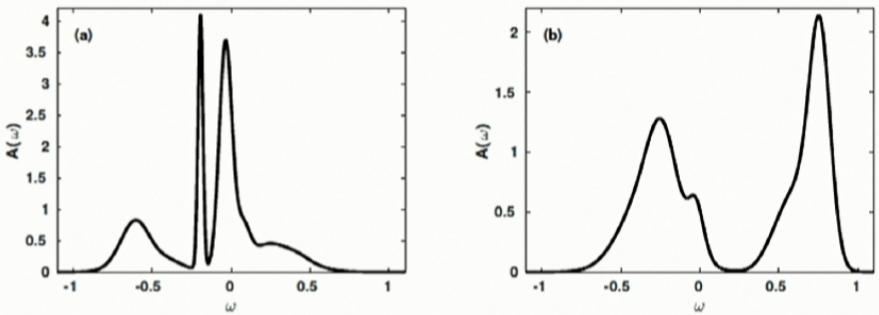
Learning and Tuning Sets



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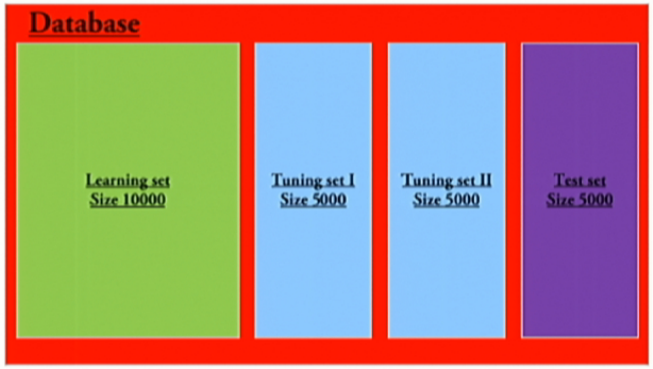

Note: learning involves fitting directly to real frequencies

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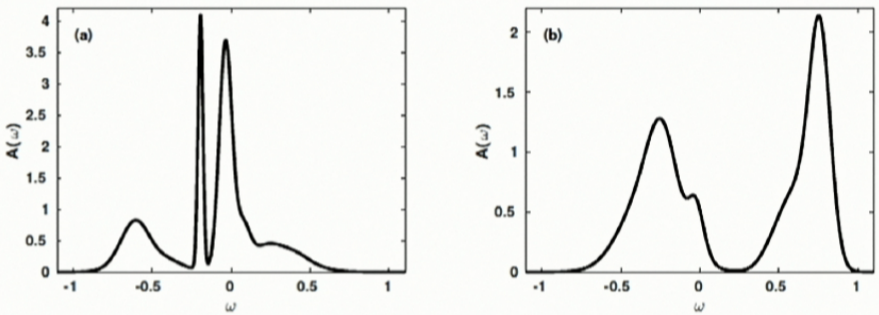
Learning and Tuning Sets



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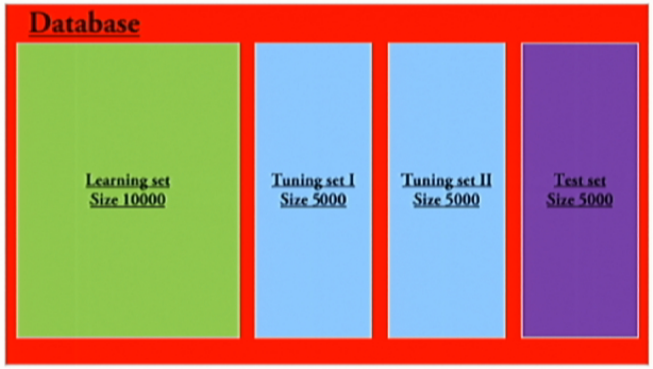

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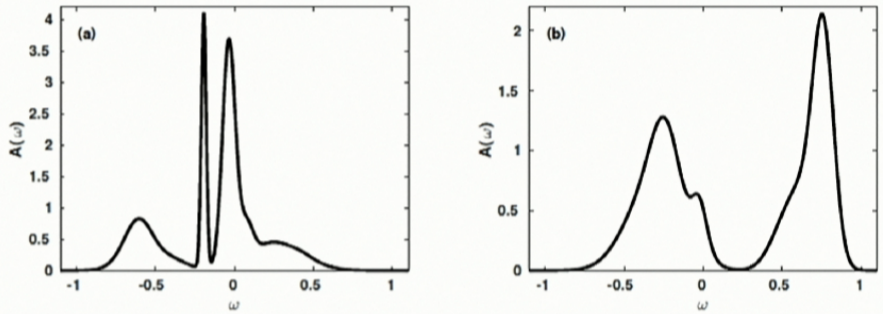
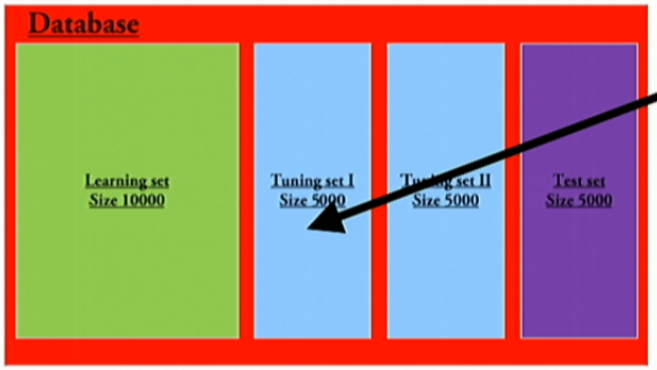


Figure 1: Two different (a) and (b) possible $A(\omega)$ in the database.

Tune hyperparameters



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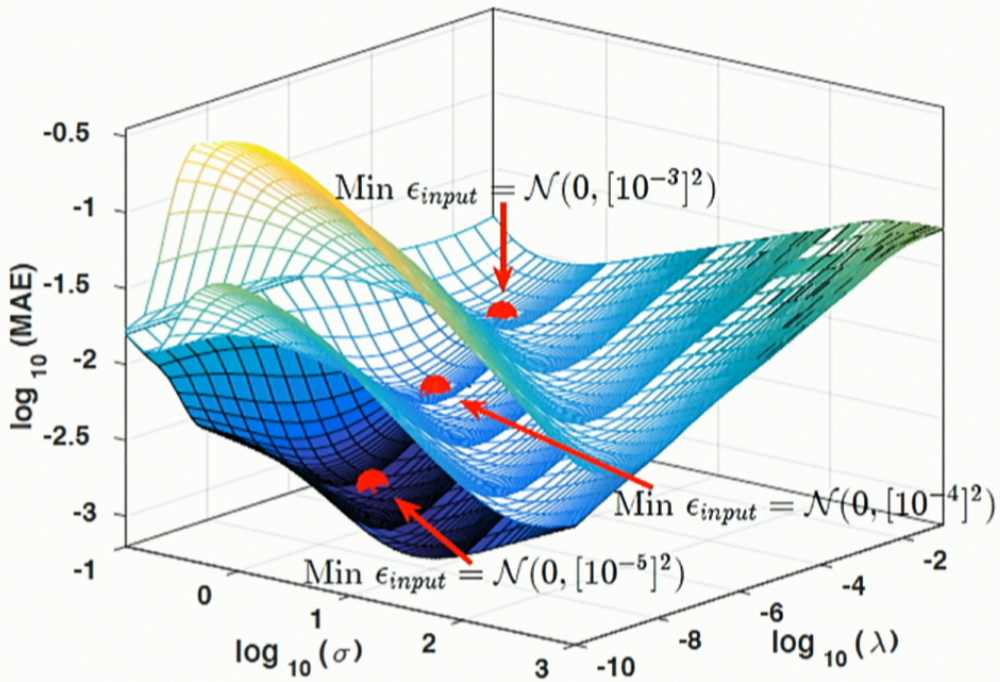
Tuning the hyperparameters (1st level regression)



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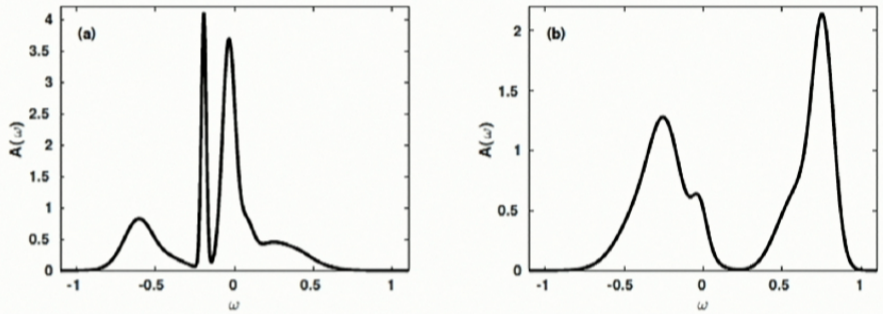

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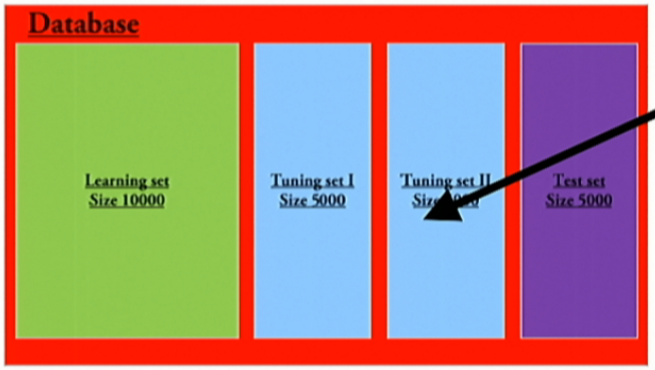

Tune covariance matrix (projection and error estimates)

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Projection

Our functions have constraints (non-negative; low order moments fixed)

Constrained regression very difficult to implement; computationally inefficient.

=> do unconstrained regression, then find function in space that satisfies constraints and is `closest' to unconstrained

$$\hat{A}_{\text{projected}} = \underset{\{A^* : A^* \text{ satisfies constraints (22) to (25)}\}}{\arg\min} \|A^* - \hat{A}\|_{\mathcal{M}}.$$

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Subtlety: some regions of frequency space are better determined than others

=> define 'distance' via (principal components of) empirical covariance matrix

$$\| \bullet \|_{\mathcal{M}} = \bullet^{\mathsf{T}} \Sigma^{-1} \bullet$$

chosen by training

$$\hat{\Sigma} = \sum_{k=1}^{p} \lambda_k \mathrm{v}_k \mathrm{v}_k^{\mathsf{T}} + \mathrm{diag}\Big(\sum_{k=p+1}^{|\{\omega\}|} \lambda_k \mathrm{v}_k \mathrm{v}_k^{\mathsf{T}} \Big)$$

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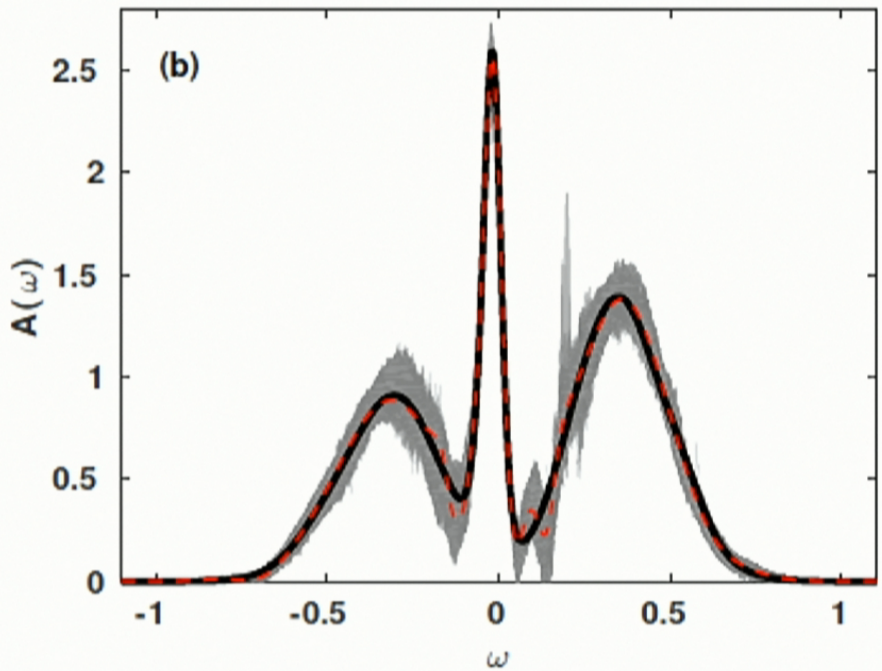
covariance matrix: also allows uncertainty estimates

90% confidence interval



Training of confidence interval done independently of regression.
Our statistician collaborators recommend 'quantile random forests'

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Error analysis: two metrics

Kubic-Leibler (minimize entropy)—
this is the metric MaxEnt optimizes

$$KL_j = \int d\omega A^j(\omega) \ln \frac{A^j(\omega)}{\hat{A}^j_{predicted}(\omega)}$$

$$MAE_j = \frac{1}{N_\omega} \sum_{i=1}^{N_\omega} \left| A^j(\omega_i) - \hat{A}^j_{predicted}(\omega_i) \right|,$$

Mean Absolute Error (minimize difference)

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Comparison to MaxEnt: modest noise

Red: statistical regression has lower error

Blue: Maxent has lower error

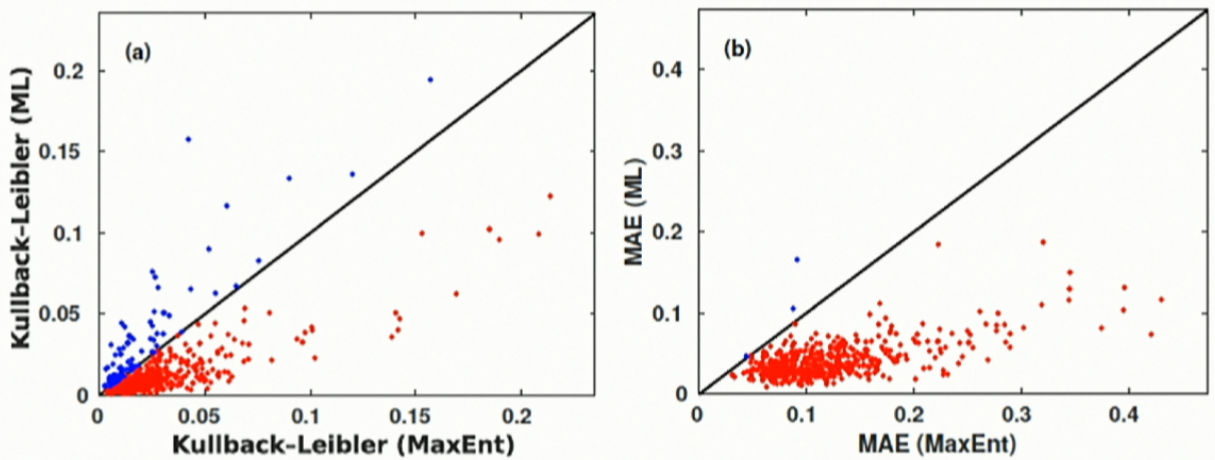

Figure 5: (Color online) Error for $\epsilon = \mathcal{N}(0, [10^{-3}]^2)$.

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Red: statistical regression has lower error

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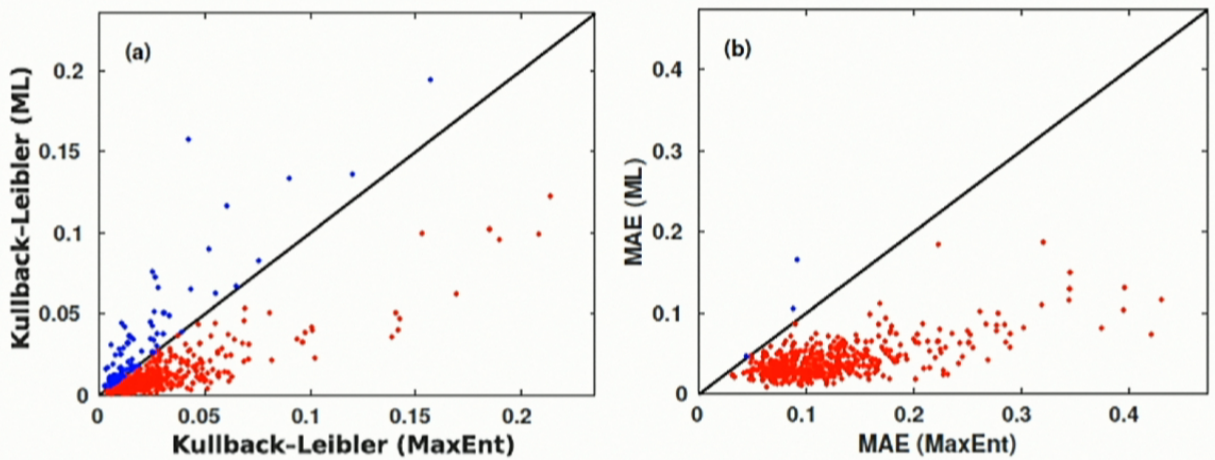

Figure 5: (Color online) Error for $\epsilon = \mathcal{N}(0, [10^{-3}]^2)$.

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Tiny noise (10^{-5})

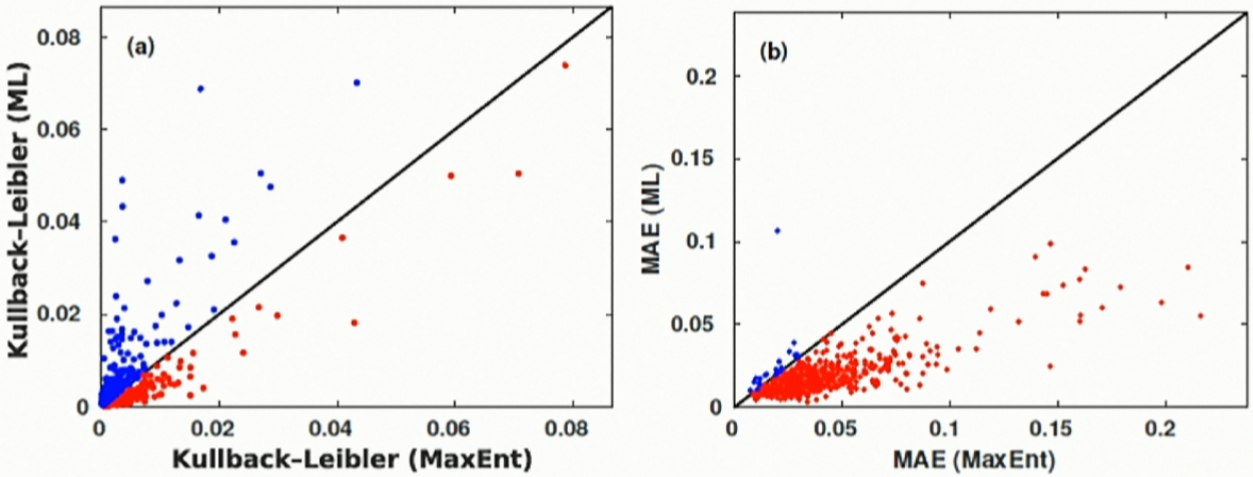

Figure 7: (Color online) Error for $\epsilon = \mathcal{N}(0, [10^{-5}]^2)$.

Only for smallest noise, and for K-L error is Max-Ent comparably good

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Continuation Conclusions

- Ill-posed inverse problem solved by statistical inference
- Method regularizes operator and provides error estimate (indep. of solution)
- A few months work produced a method comparable (better for noisy data) to Max Ent, which has had 2 decades of optimization
- Method could be useful for other inverse problems

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