The Kavli Institute for Systems Neuroscience

Centre for the biology of memory

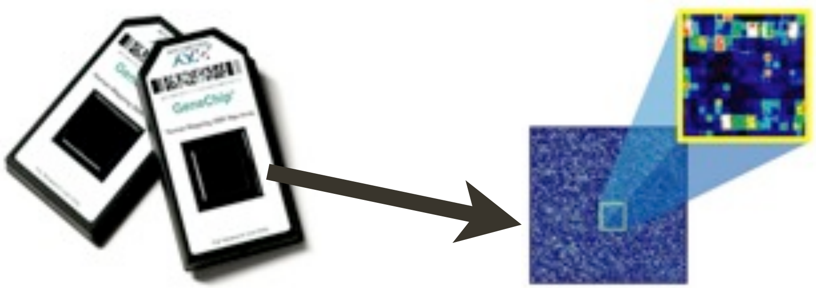
NORDITA
Nordic Institute
for Theoretical Physics

Mean Field Theory for Non-equilibrium Network Reconstruction

Yasser Roudi

Kavli Institute for Systems Neuroscience, Trondheim
NORDITA, Stockholm

~ new recording technology allows measuring the activity of many elements in a biological network.



gene microarray data

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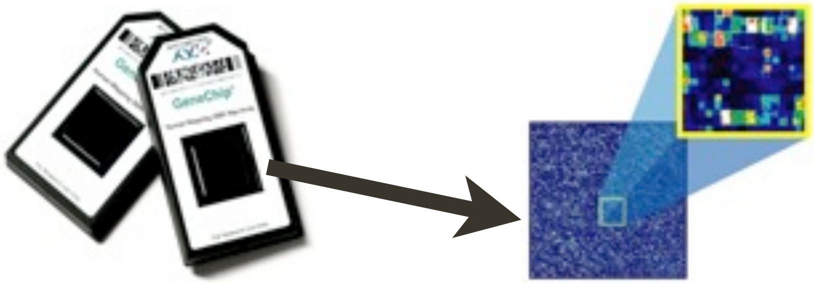

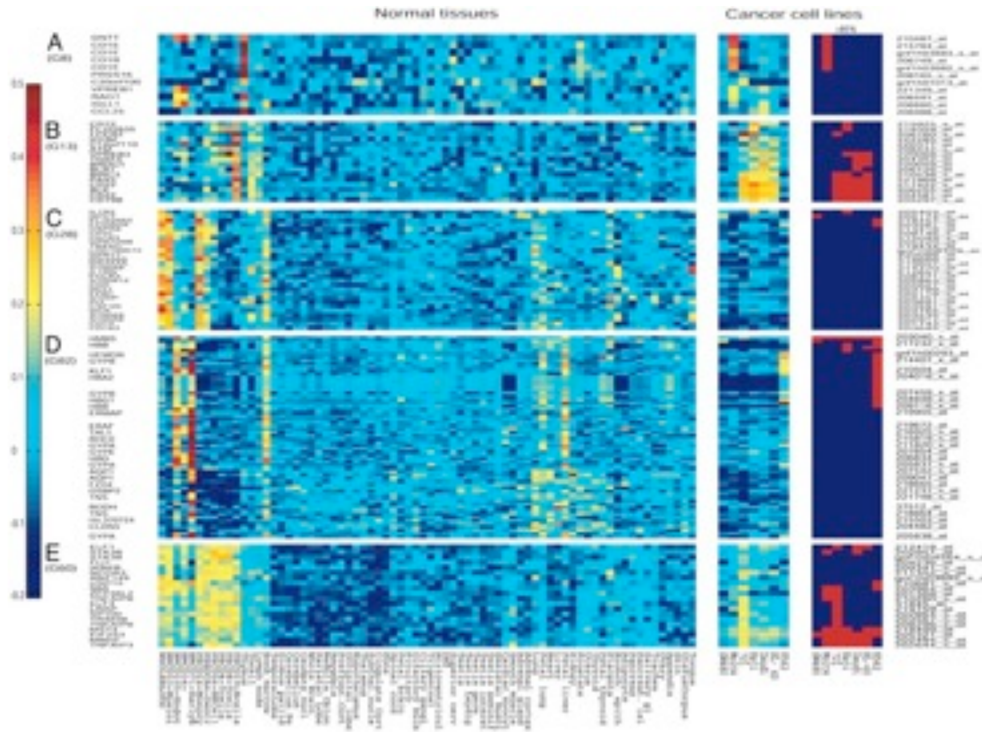

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Inverse statistical mechanics for reconstructing biological networks

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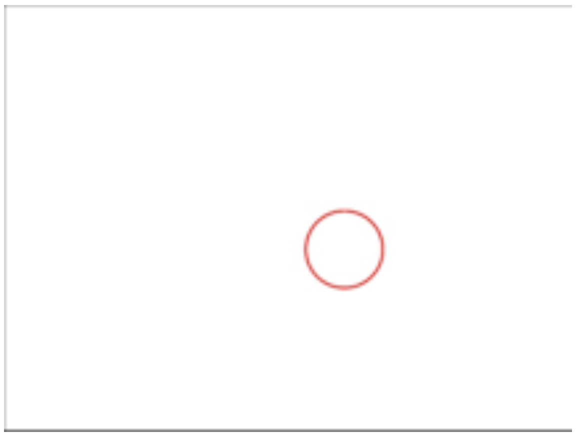

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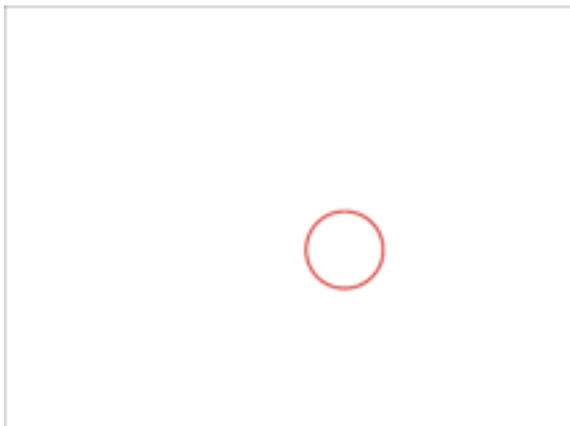

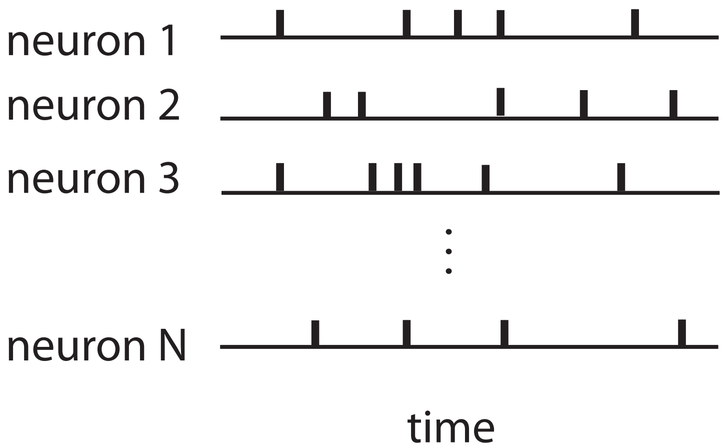

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correlation is not connection

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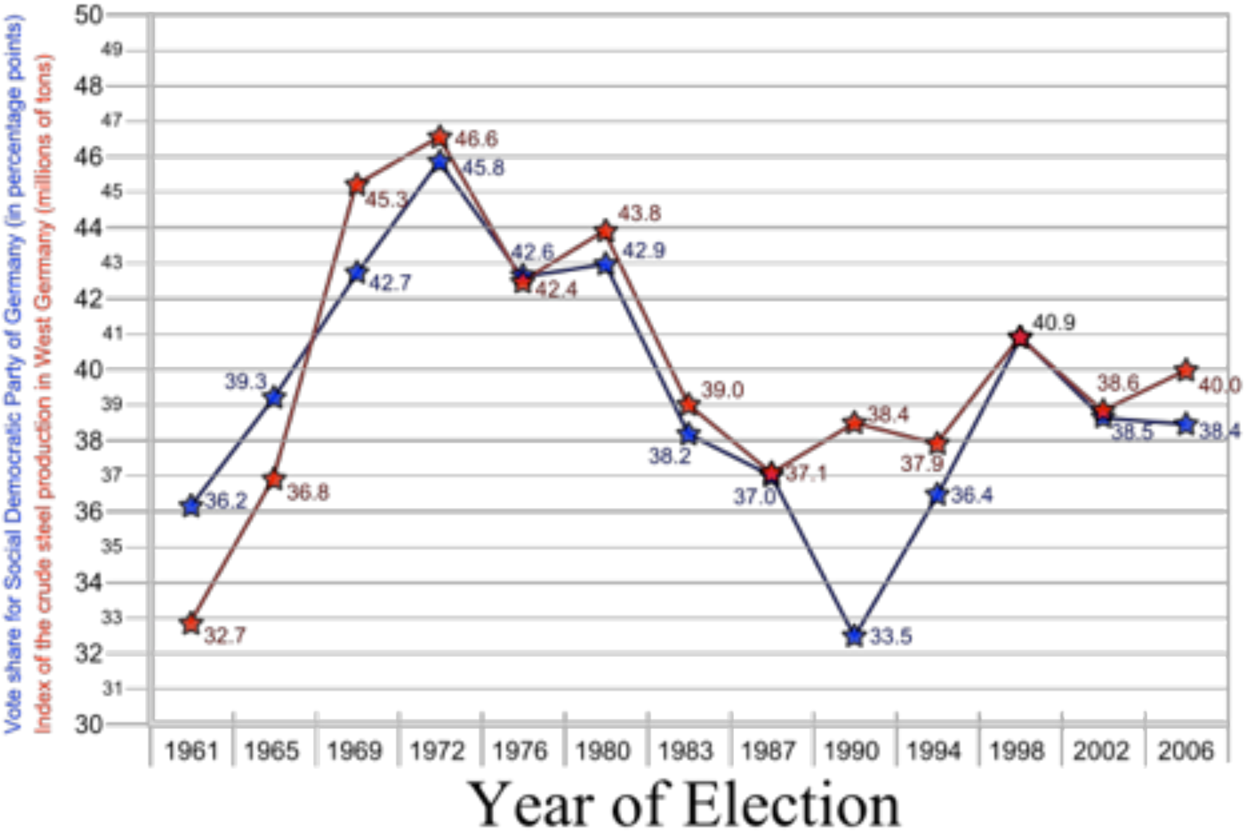

Mierscheid Law

J. M. Mierscheid (1983)

The vote share of the German Social Democratic Party (SPD) equals the index of the crude steel production in the Western federal states (Wikipedia) can we use this data to infer connections?

outline

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- equilibrium inverse Ising model for neural data and its shortcomings for neural data.

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- Mean-Field and TAP approximations for a non-equilibrium model and quantifying their errors.

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- Fitting a non-equilibrium Ising model.
- Mean-Field and TAP approximations for a non-equilibrium model and quantifying their errors.
- The non-equilibrium approach helps inferring the connectivity in a realistic simulated cortical model.

equilibrium inverse Ising problem

$$\Pr(s_1, \ldots, s_N) = \frac{1}{Z} \exp\left[\sum_i h_i s_i + \sum_{i<j} J_{ij} s_i s_j\right]$$

equilibrium inverse Ising problem

$$m_i = \langle s_i \rangle$$

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Exact method: Boltzmann learning is slow!

Fast approximate methods:

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$$h_i = \tanh^{-1} m_i - \sum_j J_{ij} m_j + m_i \sum_j J_{ij}^2 (1 - m_j^2) \quad C_{ij}^{-1} = -J_{ij} - 2J_{ij}^2 m_i m_j$$

Kappen & Rodriguez 98,
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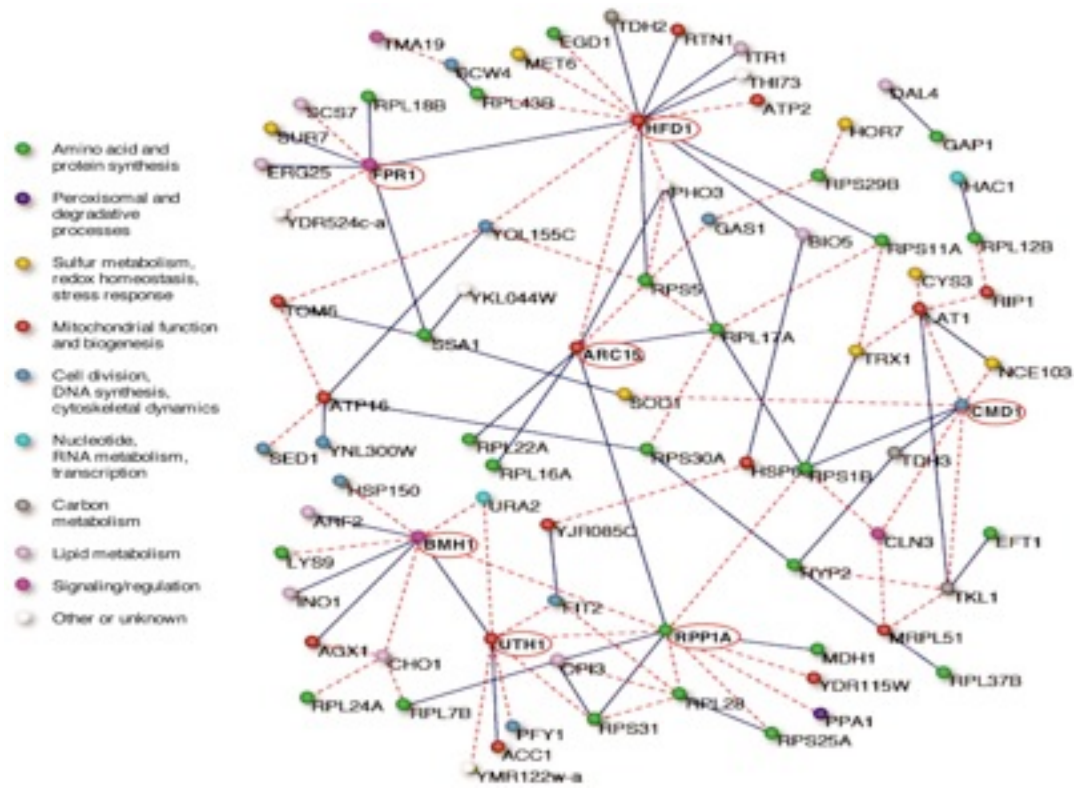
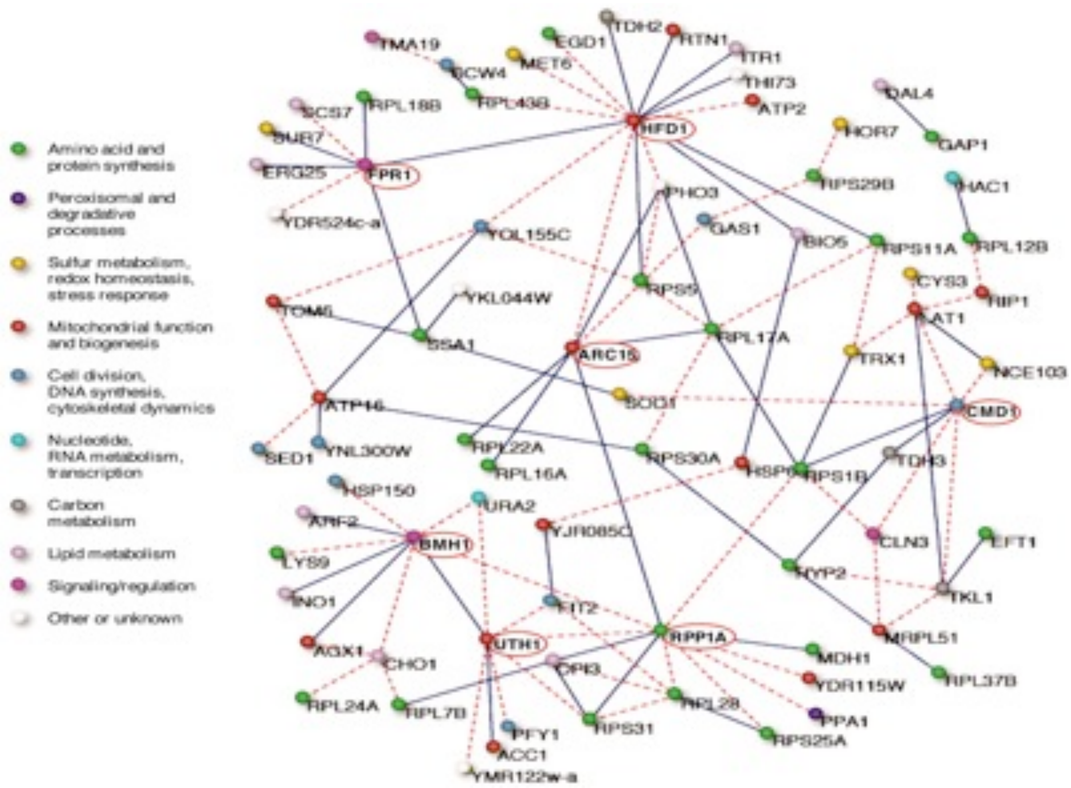
- Sessak-Monasson, SusP, independent-pair, high magnetization expansion

Sessak & Monasson 09, Mezard & Mora 09, Roudi et al 09



Lazon et al 06

microarray expression data from *Saccharomyces cerevisiae*

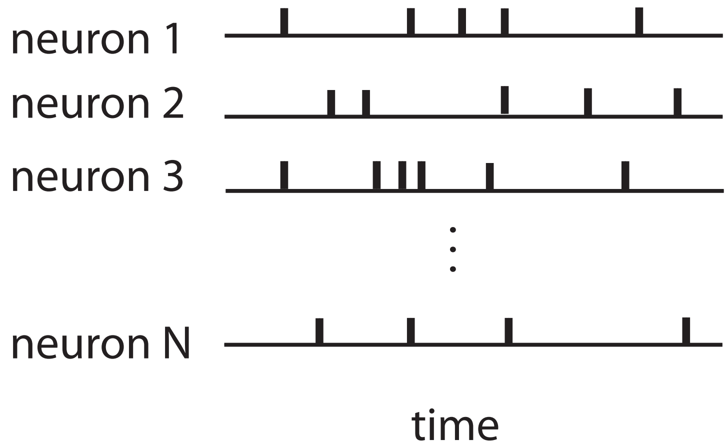


Lazon et al 06 microarray expression data from *Saccharomyces cerevisiae*

~ reconstructing protein complexes from co-evolution of contacting residues

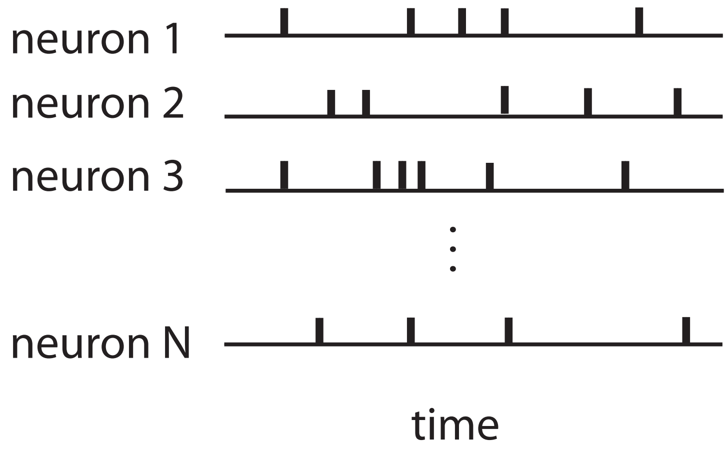
Weigt, White, Szurmant, Hoch, Hwa (PNAS 2009)

binary representation of spike trains



binary representation of spike trains

- bin the spike train



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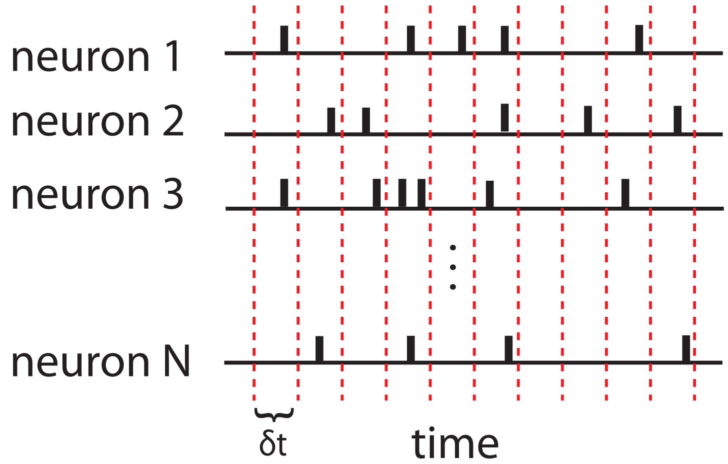

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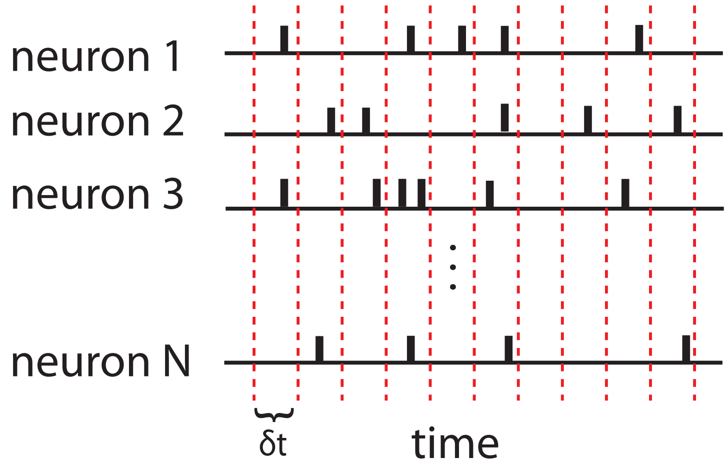

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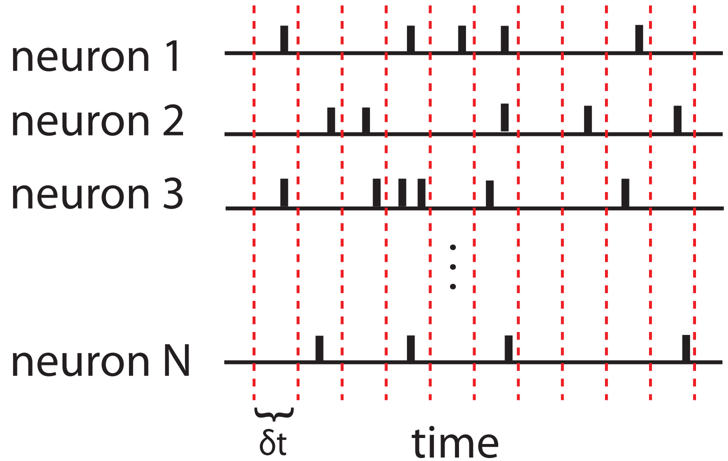

neuron 1	1	-1	-1	1	1	1	-1	-1	1	-1
neuron 2	-1	1	1	-1	-1	1	-1	1	-1	1
neuron 3	1	-1	1	1	-1	1	-1	-1	1	-1
⋮										
neuron N	-1	1	-1	1	-1	1	-1	-1	-1	1

δt time

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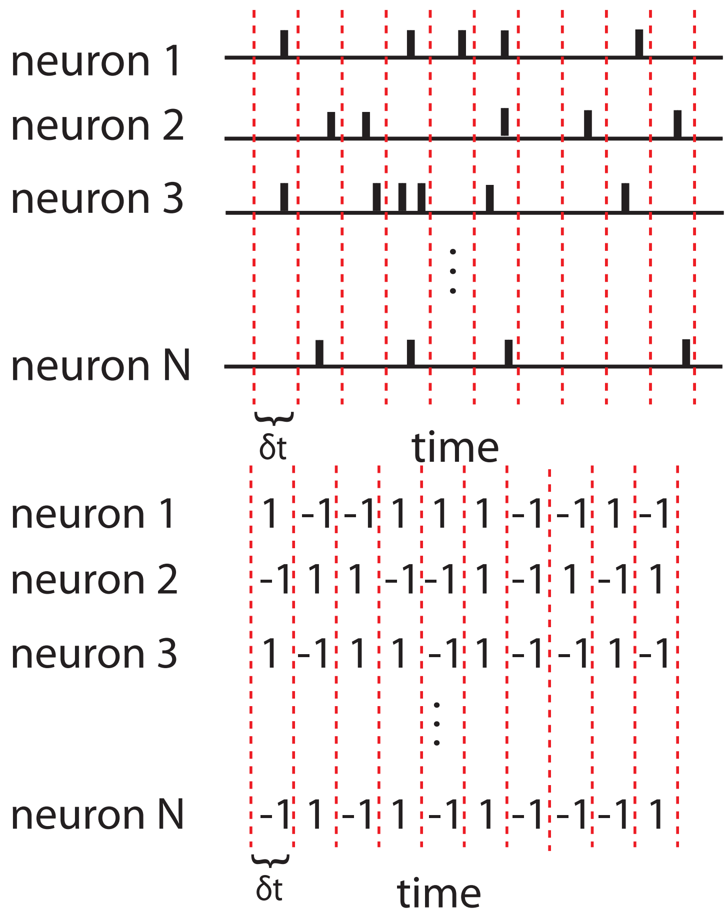

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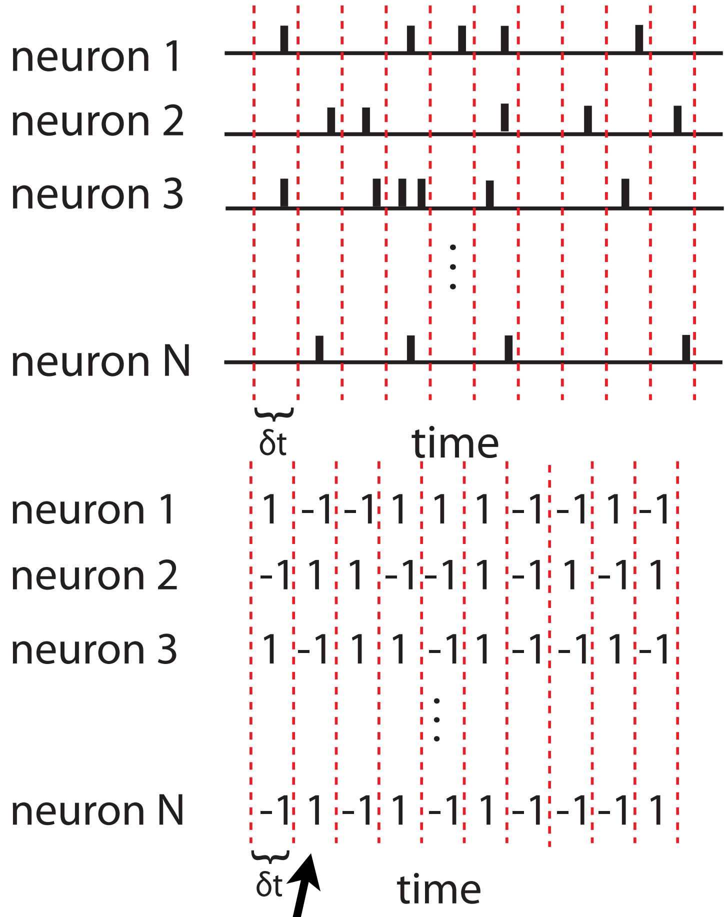

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- compute experimental means and corr.

$$\langle s_i \rangle_{\text{data}} = \frac{1}{T} \sum_t s_i(t)$$

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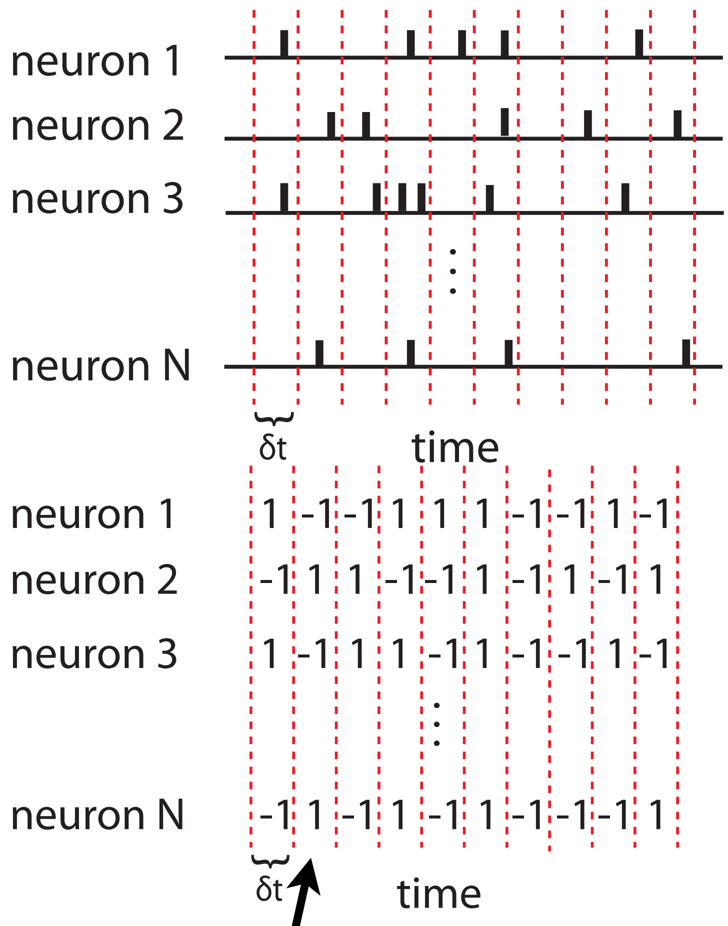

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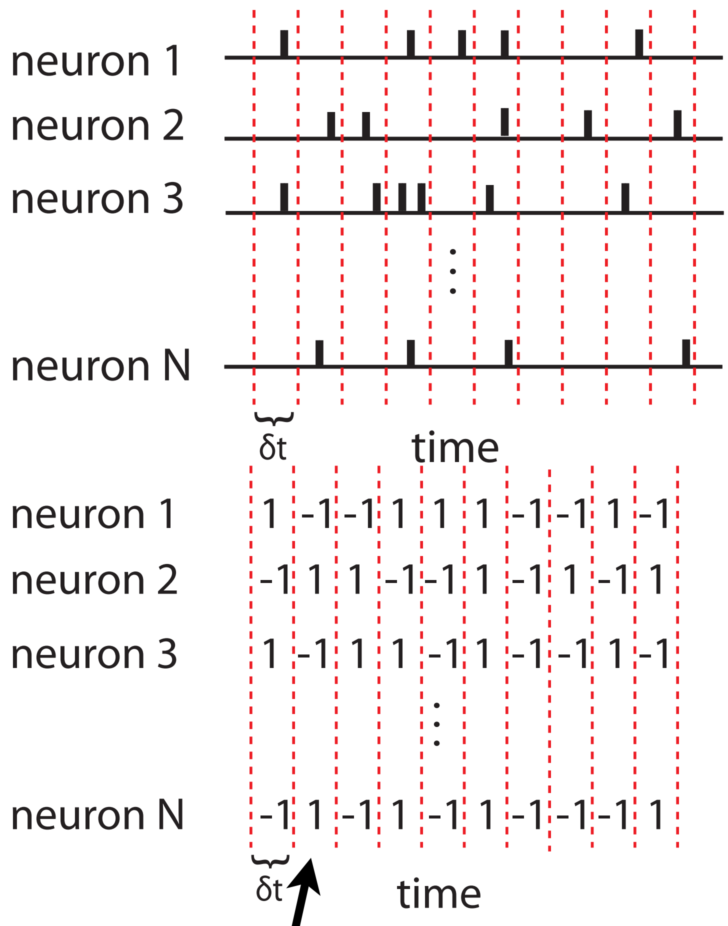
Schneidman et al 2006, Shlens et al 2006



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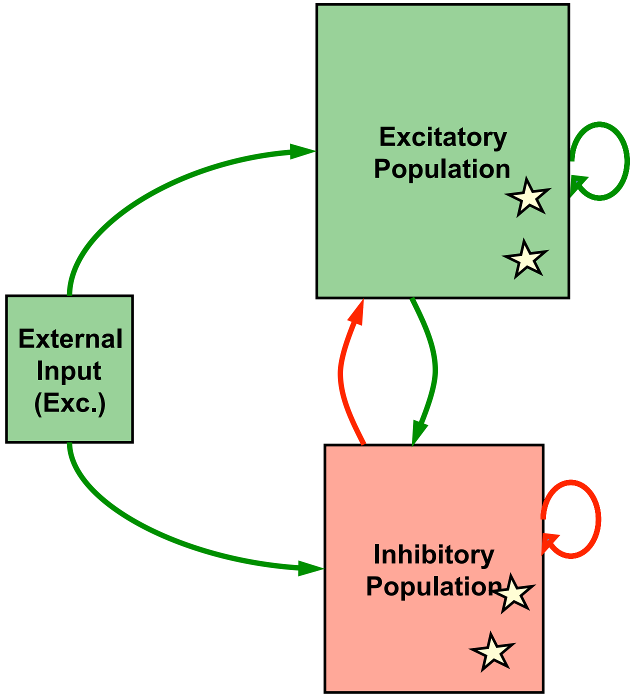
2 populations in network: Excitatory, Inhibitory

Excitatory external drive ("rest of brain")

realistic modeling: Hodgkin-Huxley-like neurons, conductance-based synapses

Probability of connection between any two neurons is c = K/N, N is the size of the population, K is the average number of presynaptic neurons.



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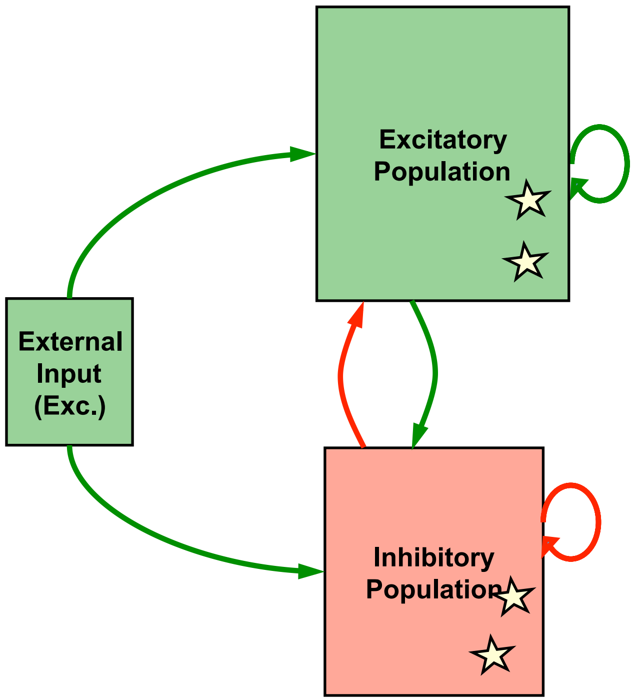
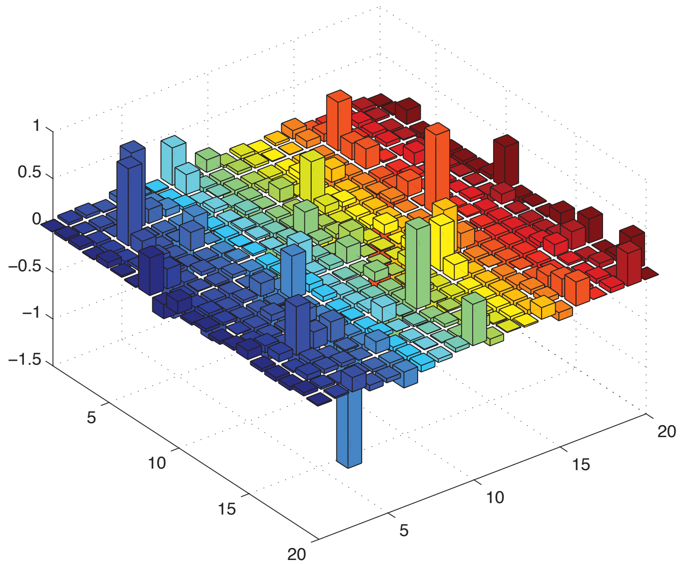


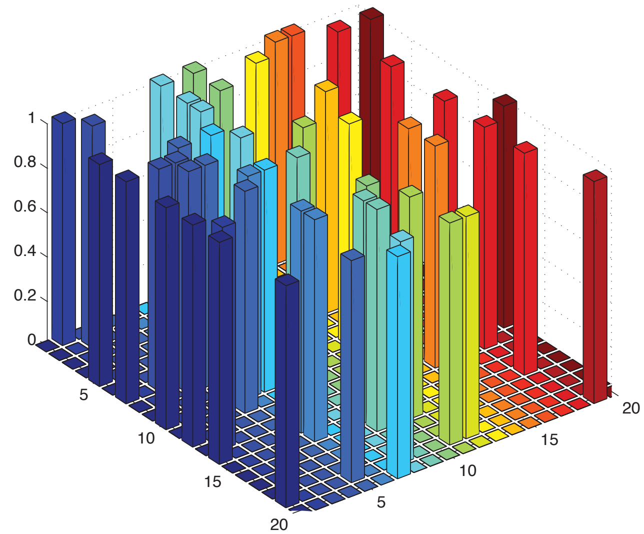
Results here for c = 0.1, N = 1000

neural data

inferred



real



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Generalised Linear models (GLM; Hawks + nonlinearity)

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Network of Integrate-Fire neurons

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synchronous discrete time

$$p_t(\mathbf{s}) = \sum_{\mathbf{s}'} W_t[\mathbf{s};\mathbf{s}'] p_{t-1}(\mathbf{s}')$$

$$W_t[\mathbf{s};\mathbf{s}'] = \prod_i \frac{\exp(s_i \theta_i(t-1))}{2\cosh(\theta_i(t-1))}$$

$$\theta_i(t) = h_i(t) + \sum_j J_{ij} s'_j(t),$$

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asynchronous, continuous time

$$\frac{d}{dt} p_t(\mathbf{s}) = \sum_i [p_t(F_i\mathbf{s}) w_i(F_i\mathbf{s};t) - p_t(\mathbf{s}) w_i(\mathbf{s};t)]$$

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exact learning by maximizing the likelihood by gradient decent

$$\delta h_i = \eta_h \frac{\partial \mathcal{L}}{\partial h_i} \qquad \delta J_{ij} = \eta_J \frac{\partial \mathcal{L}}{\partial J_{ij}}$$

$$\delta h_i(t) = \eta_h \Big\{ \langle s_i(t+1) \rangle_r - \langle \tanh[h_i(t) + \sum_k J_{ik} s_k(t))] \rangle_r] \Big\}$$

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Exact algorithm: mean square error ~ 1/L

Weak- coupling limit: $\left\langle \left(J_{ij}^{calculated} - J_{ij}^{true}\right)^2 \right\rangle = \dfrac{1}{\left(1 - m_i^2\right)L}$

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Doesn't need long Monte Carlo runs to evaluate the second term

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~ Iterative

~ L N^3 operation per learning step

Mean Field theory for the inference in this non-equilibrium model

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step 1. derive dynamical navie MF and TAP equations for the non-equilibrium Ising model

Mean Field theory for the inference in this non-equilibrium model

step I. derive dynamical navie MF and TAP equations for the non-equilibrium Ising model

step II. use these equations to relate correlations and the couplings. (no FDT for the non-equilibrium case)

Deriving dynamical naive MF and TAP equations

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Deriving dynamical naive MF and TAP equations

auxiliary field

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average over stochastic path

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average over stochastic path

$$Z[\psi, h] = \int D\boldsymbol{\theta} \left\langle \exp\Big[\sum_{i,t} \psi_i(t) s_i(t)\Big] \right\rangle \prod_{i,t} \delta\Big(\theta_i(t) - h_i(t) - \sum_j J_{ij} s_j(t)\Big)$$

$$= \int D\boldsymbol{\theta}\hat{\boldsymbol{\theta}} \left\langle \exp\Big[i \sum_{i,t} \hat{\theta}_i(t)\{\theta_i(t) - h_i(t) - \sum_j J_{ij} s_j(t)\} + \sum_{i,t} \psi_i(t) s_i(t)\Big] \right\rangle$$

Deriving dynamical naive MF and TAP equations

auxiliary field

$$Z[\psi, h] = \left\langle \exp\left[\sum_{i,t} \psi_i(t) s_i(t)\right] \right\rangle \qquad \langle s_i(t) \rangle = \lim_{\psi \to 0} \frac{\partial \log Z}{\partial \psi_i(t)}$$

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$$\Gamma[\hat{m}, m] \equiv \log Z[\psi[\hat{m}, m], h[\hat{m}, m]] - \sum_{i,t} \psi_i[\hat{m}, m](t) m_i(t) + i \sum_{i,t} h_i[\hat{m}, m](t) \hat{m}_i(t),$$

Deriving dynamical naive MF and TAP equations

auxiliary field

$$Z[\psi, h] = \left\langle \exp\left[\sum_{i,t} \psi_i(t) s_i(t)\right] \right\rangle \qquad \langle s_i(t) \rangle = \lim_{\psi \to 0} \frac{\partial \log Z}{\partial \psi_i(t)}$$

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$$\Gamma[\hat{m}, m] \equiv \log Z[\psi[\hat{m}, m], h[\hat{m}, m]] - \sum_{i,t} \psi_i[\hat{m}, m](t) m_i(t) + i \sum_{i,t} h_i[\hat{m}, m](t) \hat{m}_i(t),$$

rescale $J_{ij} \longrightarrow \alpha J_{ij}$**, expand** Γ **around** $\alpha = 0$ **and then set** $\alpha = 1$

$$\frac{\partial \Gamma}{\partial \hat{m}_i(t)} = i h_i[\hat{m}, m](t)$$

$$\frac{\partial \Gamma}{\partial \hat{m}_i(t)} = i h_i[\hat{m}, m](t)$$

asynchronous update

first order in α

$$m_i(t+1) = \tanh\left[h_i(t) + \sum_j J_{ij} m_j(t)\right]$$

second order α

$$m_i(t+1) = \tanh\left[h_i(t) + \sum_j J_{ij} m_j(t) - m_i(t+1) \sum_j J_{ij}^2 (1 - m_j^2(t))\right]$$

$$\frac{\partial \Gamma}{\partial \hat{m}_i(t)} = ih_i[\hat{m}, m](t)$$

asynchronous update

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synchronous update

$$m_i(t) + \frac{dm_i(t)}{dt} = \tanh\left[h_i(t) + \sum_j J_{ij} m_j(t)\right]$$

$$m_i(t) + \frac{dm_i(t)}{dt} = \tanh\left[h_i(t) + \sum_j J_{ij} m_j(t) - \left(m_i(t) + \frac{dm_i(t)}{dt}\right) \sum_j J_{ij}^2 (1 - m_j^2(t))\right]$$

Roudi and Hertz 2011, submitted

$$\frac{\partial \Gamma}{\partial \hat{m}_i(t)} = ih_i[\hat{m}, m](t)$$

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Roudi and Hertz 2011, submitted

for stationary state same as Kappen and Spanjer 2001

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asynchronous update

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Roudi and Hertz 2011, submitted

for stationary state same as Kappen and Spanjer 2001

similar approach can be used using MSR path integral for *p*-spin spherical model; Biroli 1999.

$$\langle J_{ij} \rangle = 0 \qquad \langle J_{ij}^2 \rangle = \frac{g^2}{N}$$ (asymmetric Sherrington-Kirkpatrick model)

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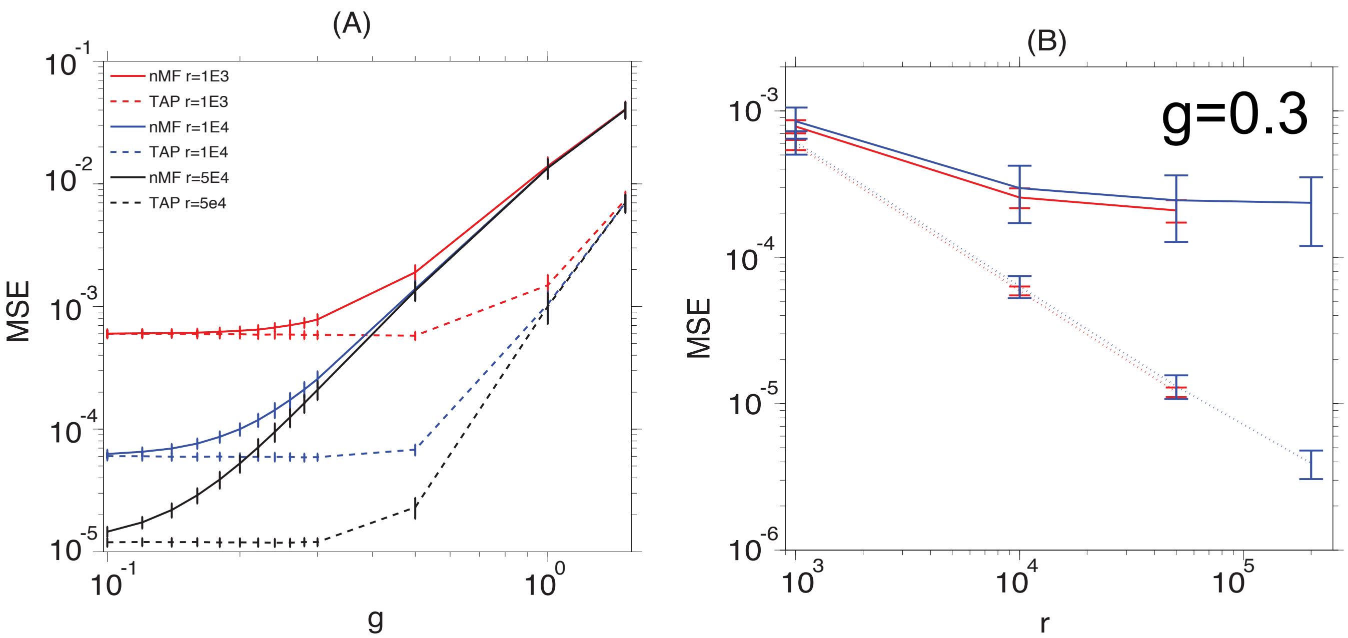
constant field



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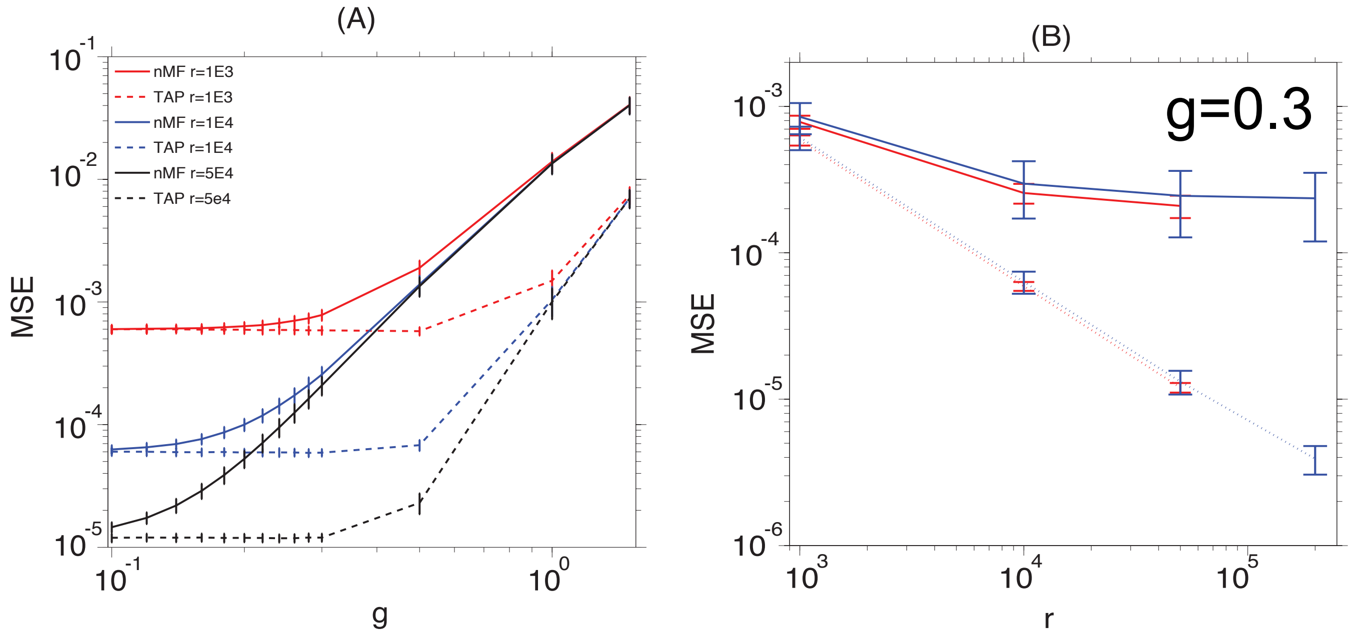
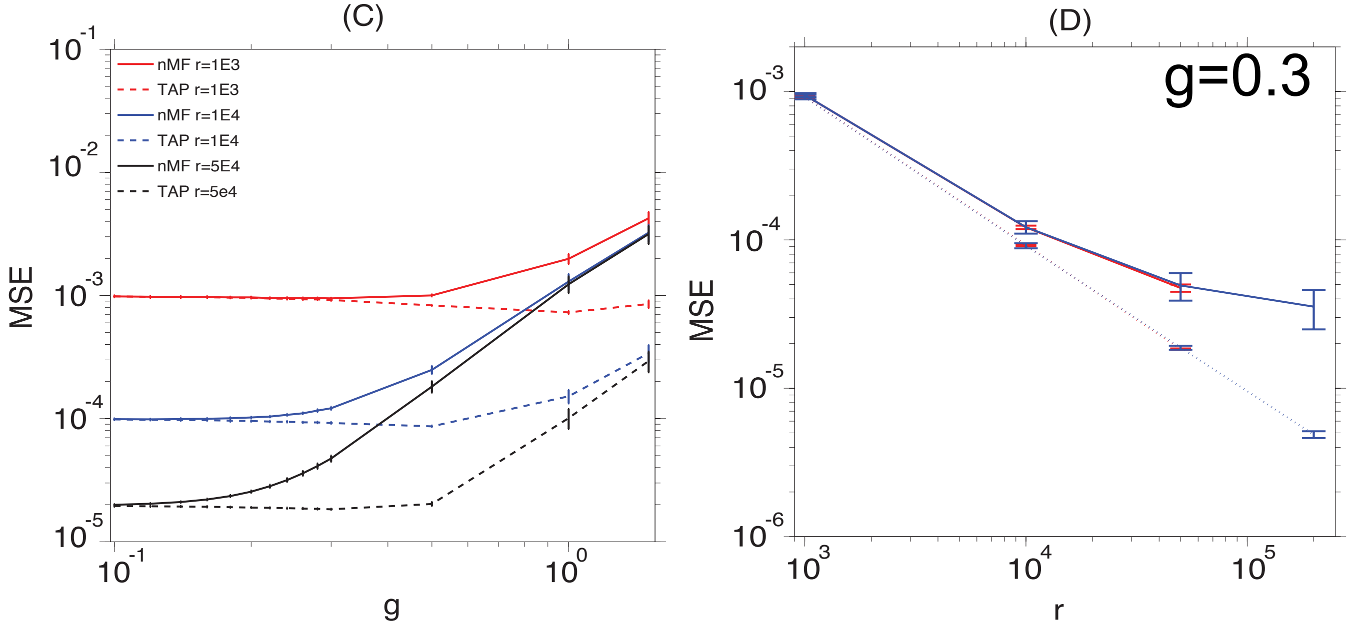


sin. field



using these forward equations for inference

I focus on stationary states first for simplicity

$$\delta J_{ij} = \eta_J \Big\{ \big\langle s_i(t+1) s_j(t) \big\rangle - \langle \tanh[h_i(t) + \sum_k J_{ik} s_k(t)] s_j(t) \rangle \Big\}$$

$$\delta J_{ij} = \eta_J \left\{ \langle s_i(t+1) s_j(t) \rangle - \langle \tanh[h_i(t) + \sum_k J_{ik} s_k(t)] s_j(t) \rangle \right\}$$

after the learning is converged $\delta J_{ij} = 0$

$$\langle s_i(t+1) s_j(t) \rangle = \langle \tanh[h_i(t) + \sum_k J_{ik} s_k(t)] s_j(t) \rangle$$

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$$S_i = m_i + \delta S_i$$

$$m_i = \langle s_i \rangle$$

$$\delta J_{ij} = \eta_J \Big\{ \langle s_i(t+1) s_j(t) \rangle - \langle \tanh[h_i(t) + \sum_k J_{ik} s_k(t)] s_j(t) \rangle \Big\}$$

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$$S_i = m_i + \delta S_i$$
$$m_i = \langle s_i \rangle$$

expanding 1st order in δs and assuming $m_i = \tanh(h_i + \sum_j J_{ik}^{\mathrm{MF}} m_k)$

$$\delta J_{ij} = \eta_J \{ \langle s_i(t+1) s_j(t) \rangle - \langle \tanh[h_i(t) + \sum_k J_{ik} s_k(t)] s_j(t) \rangle \}$$

after the learning is converged $\delta J_{ij} = 0$

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expanding 1st order in δs and assuming $m_i = \tanh(h_i + \sum_j J_{ik}^{\mathrm{MF}} m_k)$

$$\langle \delta s_i(t+1) \delta s_j(t) \rangle = (1 - m_i^2) \sum_k J_{ik}^{\mathrm{MF}} \langle \delta s_k(t) \delta s_j(t) \rangle.$$

$$\delta J_{ij} = \eta_J \{ \langle s_i(t+1) s_j(t) \rangle - \langle \tanh[h_i(t) + \sum_k J_{ik} s_k(t)] s_j(t) \rangle \}$$

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$$\langle s_i(t+1) s_j(t) \rangle = \langle \tanh[h_i(t) + \sum_k J_{ik} s_k(t)] s_j(t) \rangle$$

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$$\langle \delta s_i(t+1) \delta s_j(t) \rangle = (1 - m_i^2) \sum_k J_{ik}^{\mathrm{MF}} \langle \delta s_k(t) \delta s_j(t) \rangle.$$

$$\mathsf{J}^{\mathrm{MF}} = \mathsf{A}^{-1} \mathsf{D} \mathsf{C}^{-1}$$

$$C_{ij} = \langle \delta s_i(t) \delta s_j(t) \rangle \qquad D_{ij} = \langle \delta s_i(t+1) \delta s_j(t) \rangle$$

$$A_{ij} = (1 - m_i^2) \delta_{ij}$$

$$\delta J_{ij} = \eta_J \{ \langle s_i(t+1) s_j(t) \rangle - \langle \tanh[h_i(t) + \sum_k J_{ik} s_k(t)] s_j(t) \rangle \}$$

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expanding 3rd order in δs and assuming

$$\delta J_{ij} = \eta_J \{ \langle s_i(t+1) s_j(t) \rangle - \langle \tanh[h_i(t) + \sum_k J_{ik} s_k(t)] s_j(t) \rangle \}$$

after the learning is converged $\delta J_{ij} = 0$

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expanding 3rd order in δs and assuming

$$m_i = \tanh[h_i + \sum_k J^{\mathrm{TAP}}_{ik} m_k - m_i \sum_k (J^{\mathrm{TAP}})^2_{ik} (1 - m_k^2)]$$

$$\delta J_{ij} = \eta_J \{ \langle s_i(t+1) s_j(t) \rangle - \langle \tanh[h_i(t) + \sum_k J_{ik} s_k(t)] s_j(t) \rangle \}$$

after the learning is converged $\delta J_{ij} = 0$

$$\langle s_i(t+1) s_j(t) \rangle = \langle \tanh[h_i(t) + \sum_k J_{ik} s_k(t)] s_j(t) \rangle$$

$S_i = m_i + \delta S_i$

$m_i = \langle s_i \rangle$

expanding 3rd order in δs and assuming

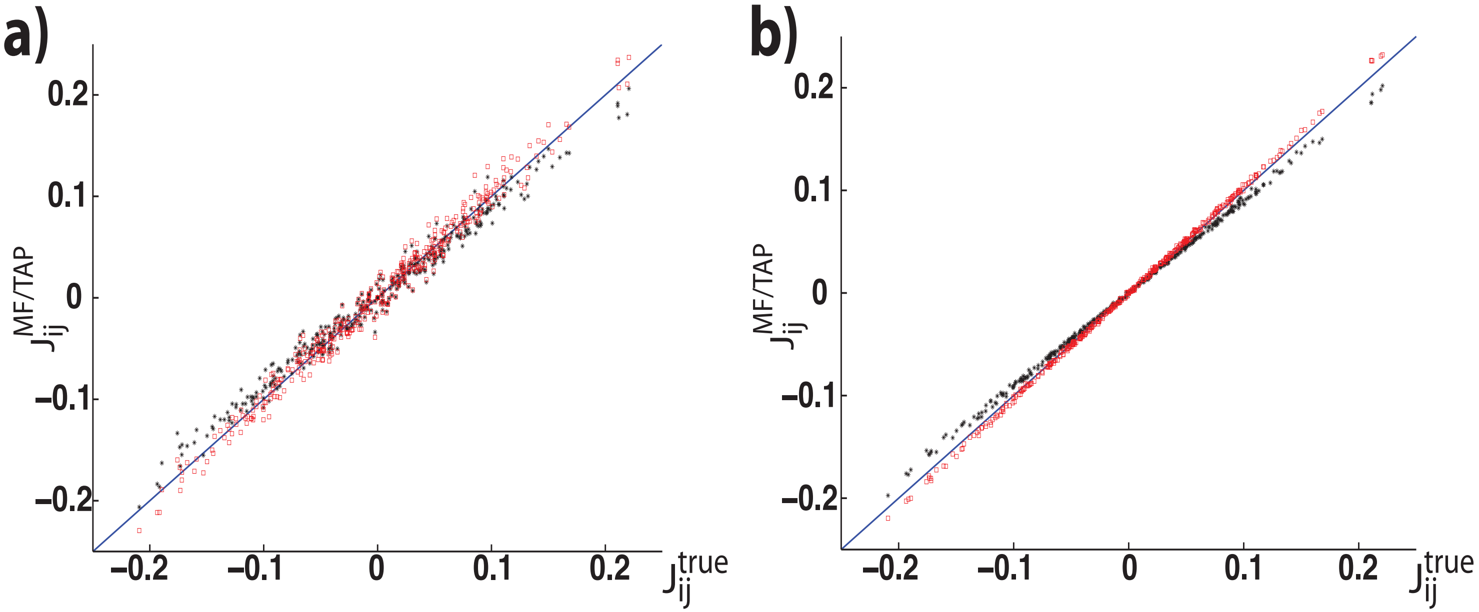
$$m_i = \tanh[h_i + \textstyle\sum_k J_{ik}^{\mathrm{TAP}} m_k - m_i \sum_k (J^{\mathrm{TAP}})_{ik}^2 (1 - m_k^2)]$$

$$J_{ij}^{\mathrm{TAP}} = {\mathrm{A}^{\mathrm{TAP}}}^{-1} \, \mathrm{DC}^{-1} = J_{ij}^{\mathrm{MF}} / (1 - F_i)$$

$$A_{ii}^{\mathrm{TAP}} = (1 - m_i^2)(1 - F_i), \qquad F_i(1 - F_i^2) = (1 - m_i^2) \sum_j (J^{\mathrm{MF}})_{ij}^2 (1 - m_j^2).$$

$$C_{ij} = \langle \delta s_i(t) \delta s_j(t) \rangle \qquad D_{ij} = \langle \delta s_i(t+1) \delta s_j(t) \rangle$$

MF and TAP tested on data generated from a kinetic Ising model:



$L = 10^4$ $L = 10^6$

L time steps, generated by a model with random couplings:

$$\langle J_{ij} \rangle = 0 \qquad \langle J_{ij}^2 \rangle = \frac{g^2}{N}$$ (asymmetric Sherrington-Kirkpatrick model)

quantifying the errors

exact algorithm is satisfied when

$$D_{ij} = \langle \tanh[h_i(t) + \sum_k J_{ik} s_k(t)] s_j(t) \rangle$$

quantifying the errors

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$$D_{ij} = \langle \tanh[h_i(t) + \sum_k J_{ik} s_k(t)] s_j(t) \rangle$$

at zero field $$D_{in} = \sum_k J_{ik} \langle s_k s_n \rangle - \tfrac{1}{3} \sum_{klm} J_{ik} J_{il} J_{im} \langle s_k s_l s_m s_n \rangle + \cdots$$

quantifying the errors

exact algorithm is satisfied when

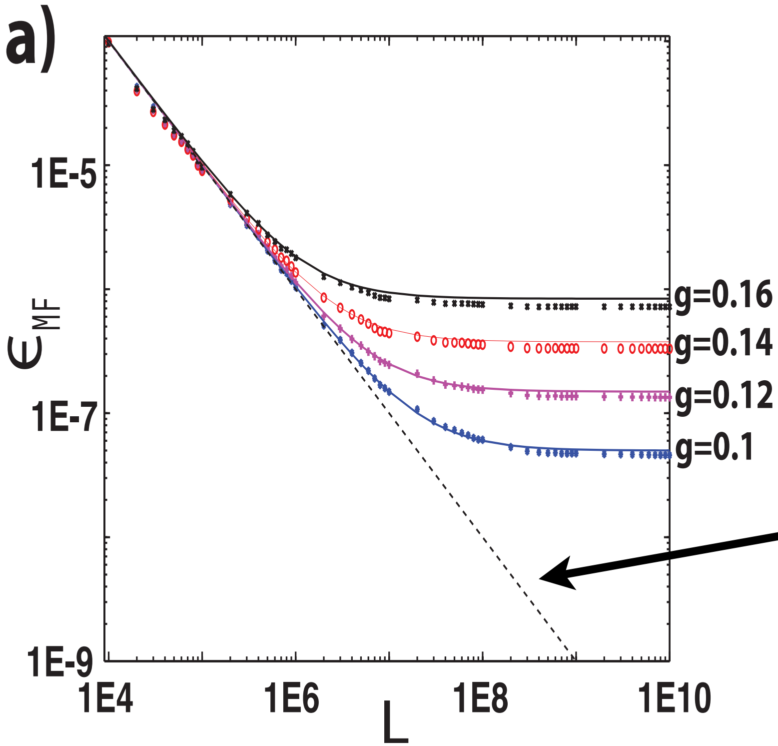
$$D_{ij} = \langle \tanh[h_i(t) + \sum_k J_{ik} s_k(t)] s_j(t) \rangle$$

at zero field $$D_{in} = \sum_k J_{ik} \langle s_k s_n \rangle - \tfrac{1}{3} \sum_{klm} J_{ik} J_{il} J_{im} \langle s_k s_l s_m s_n \rangle + \cdots$$

using $\mathsf{J}^{\mathrm{MF}} = \mathsf{A}^{-1} \mathsf{D} \mathsf{C}^{-1}$ yields $J_{ij}^{\mathrm{MF}} = J_{ij} - \sum_k J_{ik}^2 J_{ij}$

$$\left\langle \left(J_{ij} - J_{ij}^{MF} \right)^2 \right\rangle = \left\langle \sum\nolimits_k J_{ik}^2 \right\rangle^2 \left\langle J_{ij}^2 \right\rangle = \left(g^2 \right)^2 \cdot \frac{g^2}{N}$$

$$= \frac{g^6}{N}$$



MF error

error of the exact algorithm

TAP error

$$4g^{10}/N.$$

TAP error

$$4g^{10}/N.$$

much smaller than what simulations show

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much smaller than what simulations show

$$4g^{10}/N + (20g^6)/(3N^3).$$

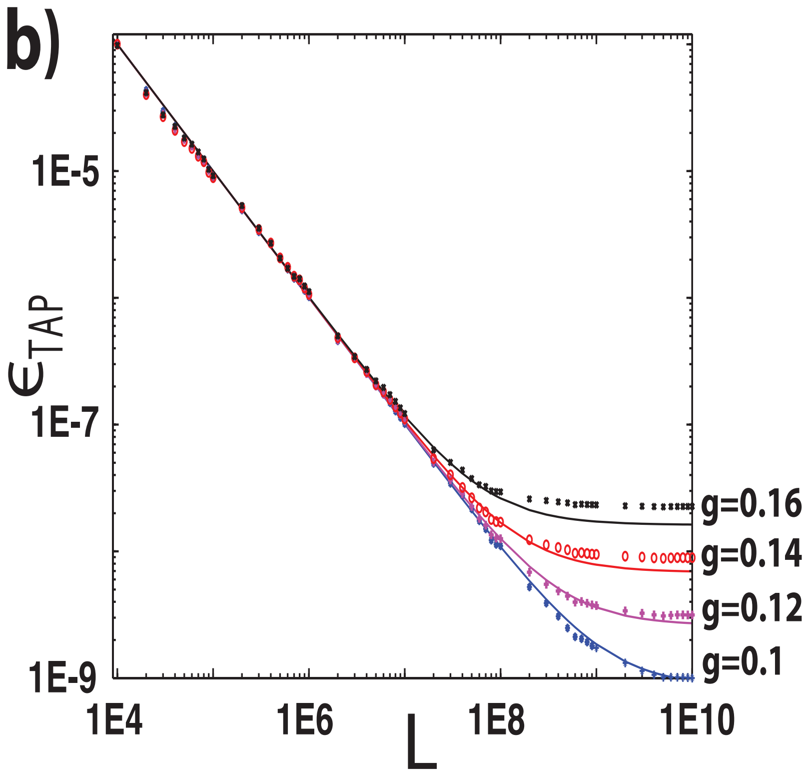
finite size effect

negligible only for N>>1/g^2

TAP error

$$4g^{10}/N.$$

much smaller than what simulations show

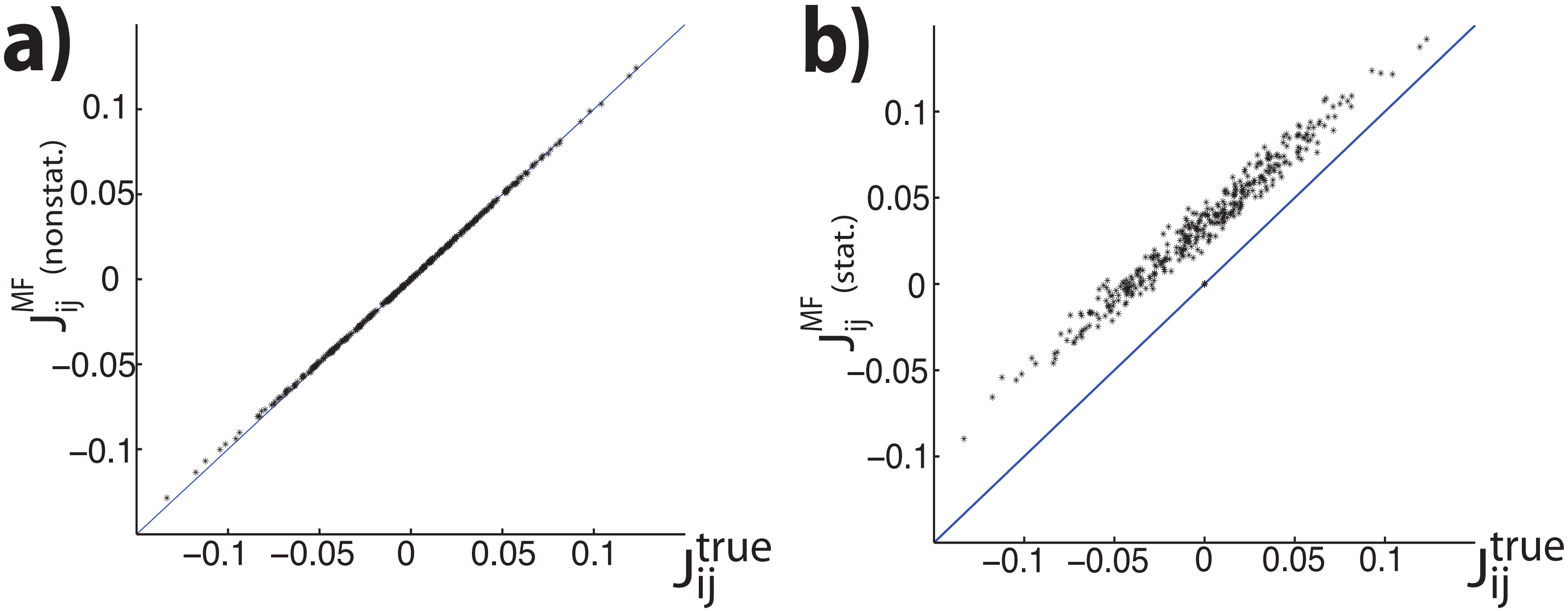


$$4g^{10}/N + (20g^6)/(3N^3).$$

finite size effect
negligible only for N>>1/g^2

Non-stationary case

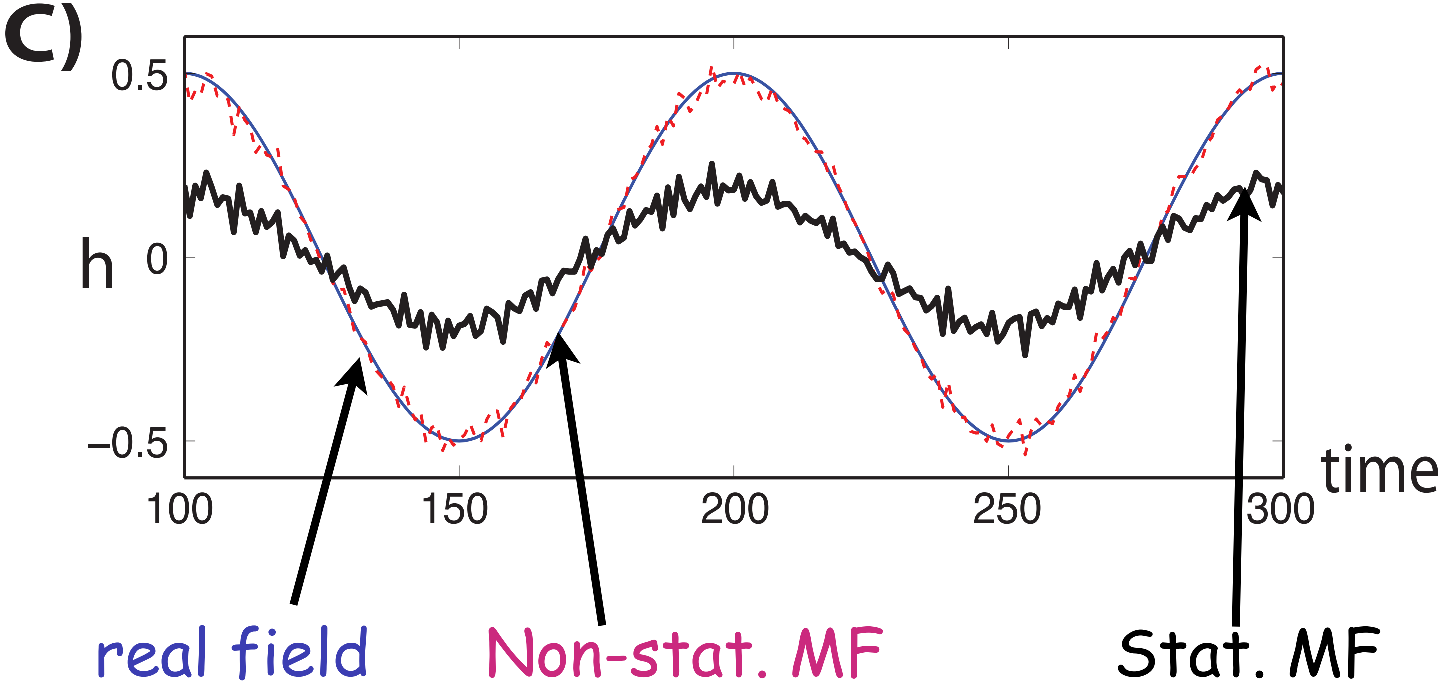
sinusoidal field applied to all spins



nonstationary MF inference applied to nonstationary data

stationary MF inference applied to nonstationary data after we inferred the couplings, we can infer the fields

$$m_i(t+1) = \tanh[h_i(t) + \sum_j J_{ij}^{\mathrm{MF}} m_j(t)].$$



simplified model of circuitry in a small (~0.5 mm) region of neocortex

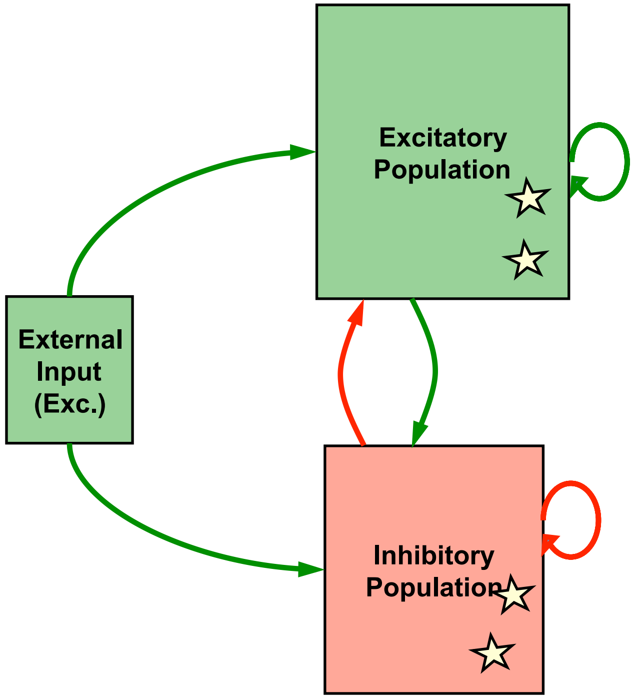
2 populations in network:
Excitatory, Inhibitory

Excitatory external drive (“rest of brain”)

realistic modeling: Hodgkin-Huxley-like neurons, conductance-based synapses

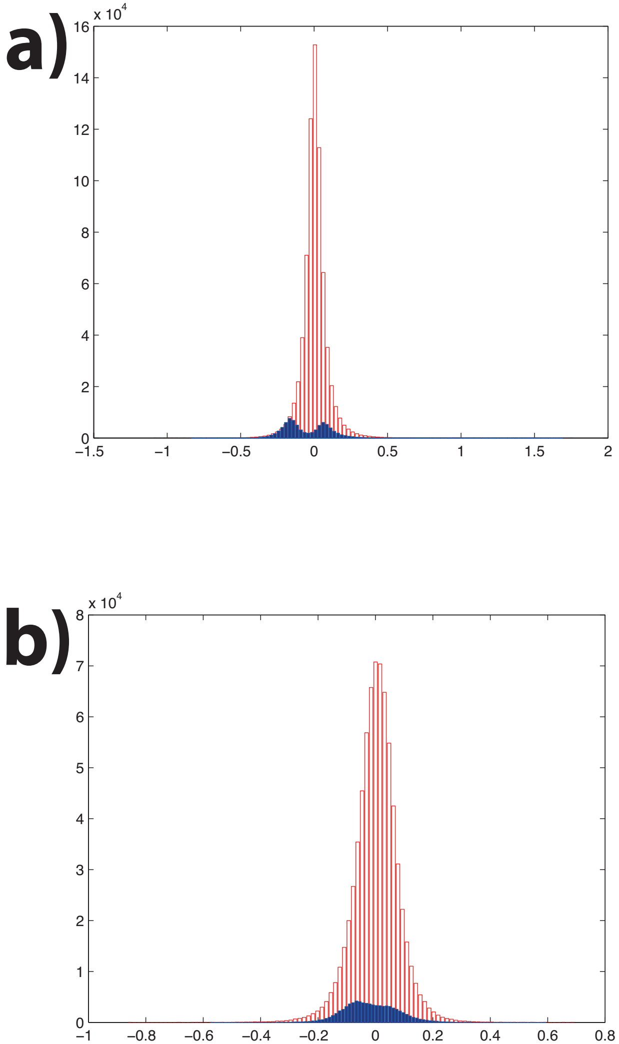
Random connectivity:
Probability of connection between any two neurons is c = K/N, N is the size of the population, K is the average number of presynaptic neurons.

Results here for
c = 0.1, N = 1000



non-
equilibrium

equilibrium



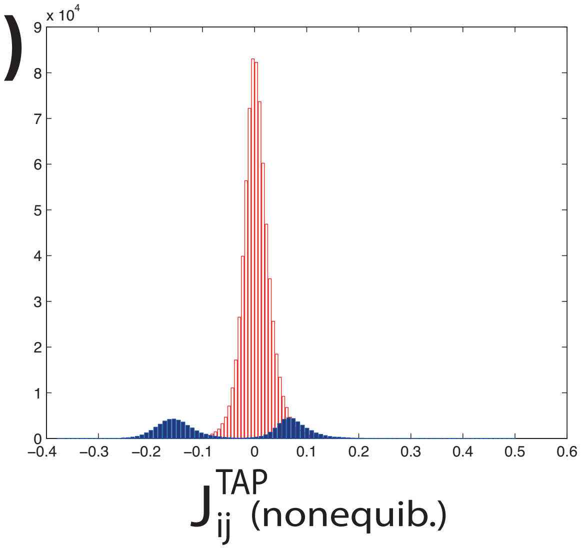
--- : synaptic connection present in original network

--- : synaptic connection absent in original network

L=10000

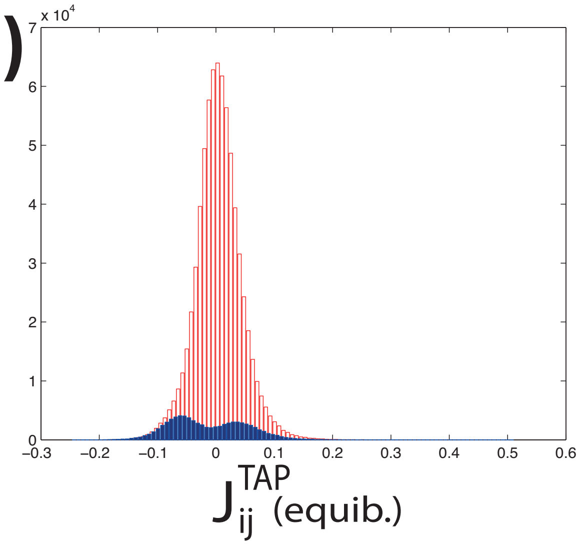
non-
equilibrium

c)



equilibrium

d)

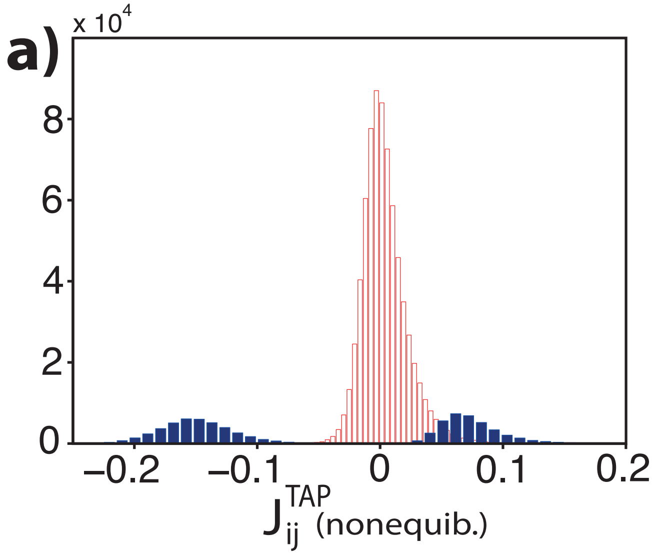


--- : synaptic connection present in original network

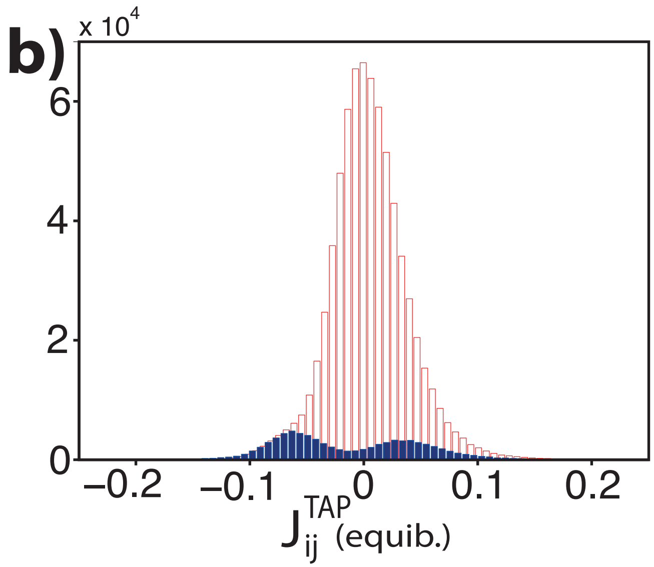
--- : synaptic connection absent in original network

L=100000

non-
equilibrium



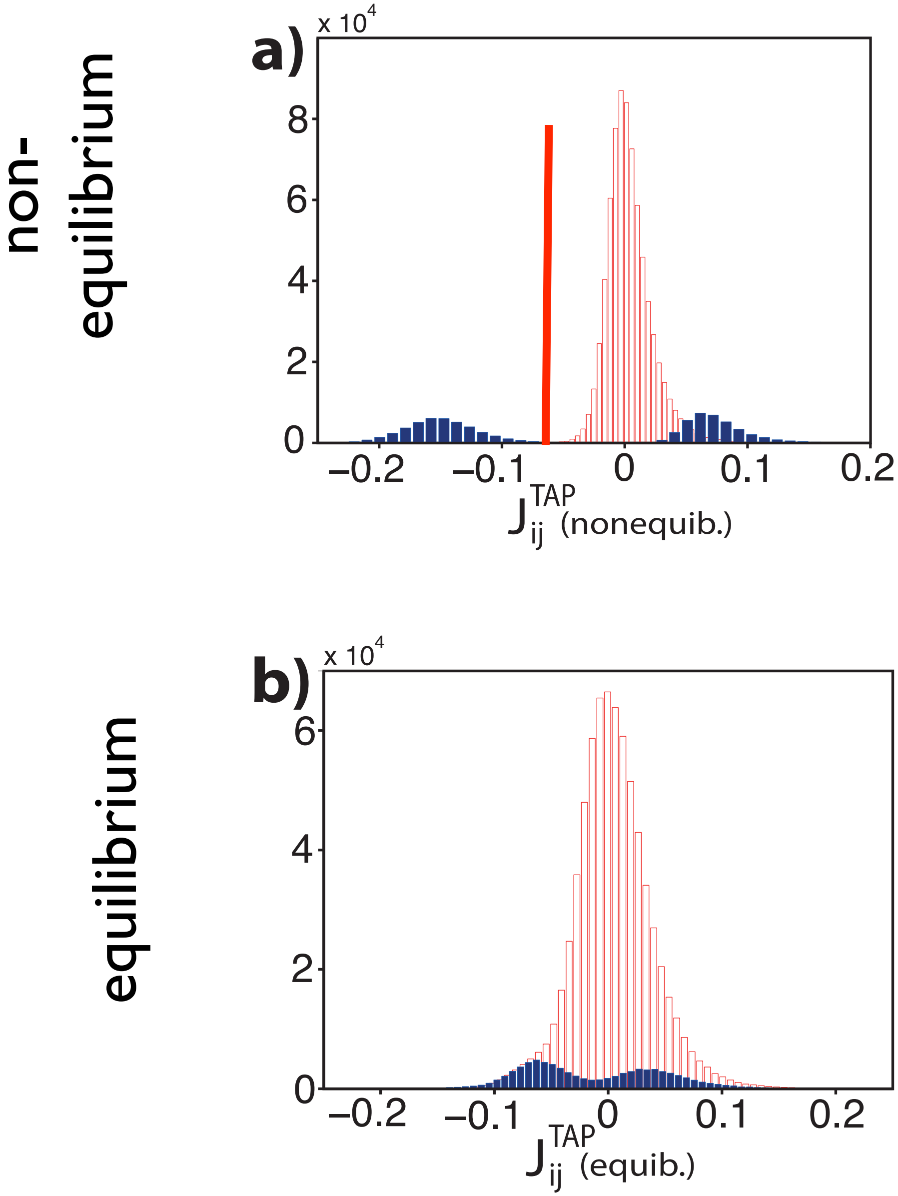
equilibrium



L=1000000

--- : synaptic connection present in original network

--- : synaptic connection absent in original network



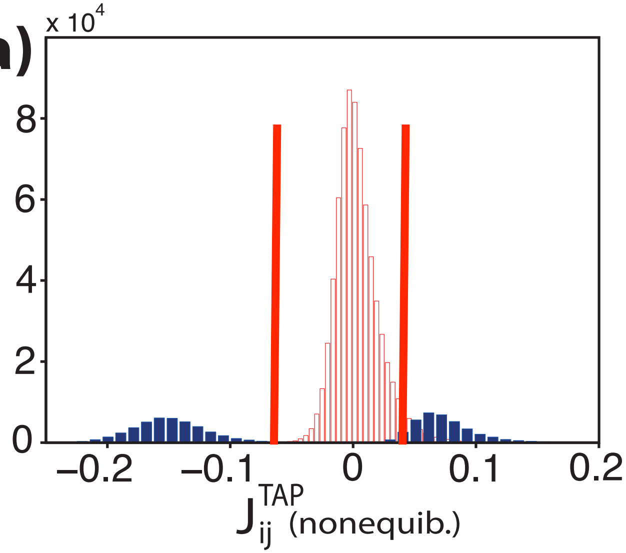
--- : synaptic connection present in original network

--- : synaptic connection absent in original network

L=1000000

non-equilibrium

a)



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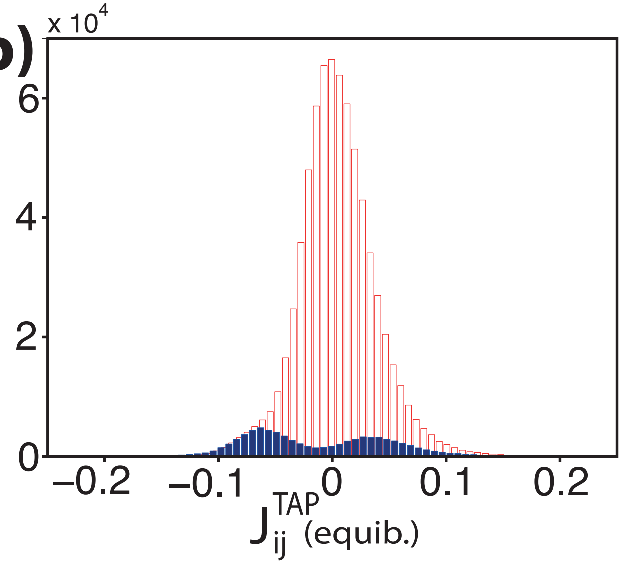
--- : synaptic connection absent in original network

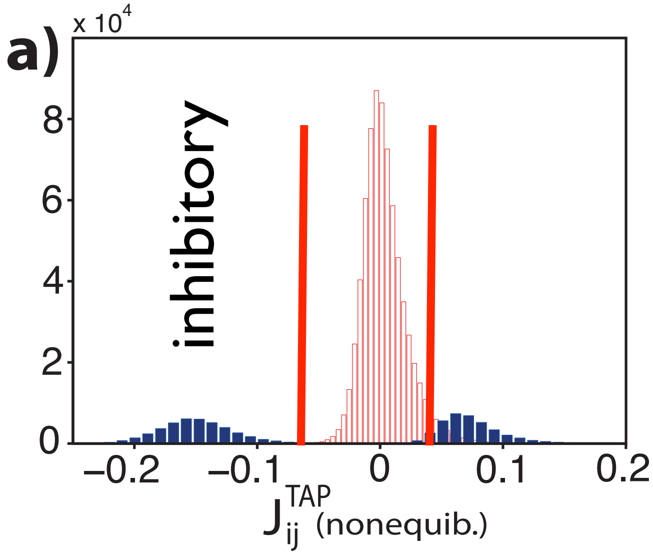
equilibrium

b)

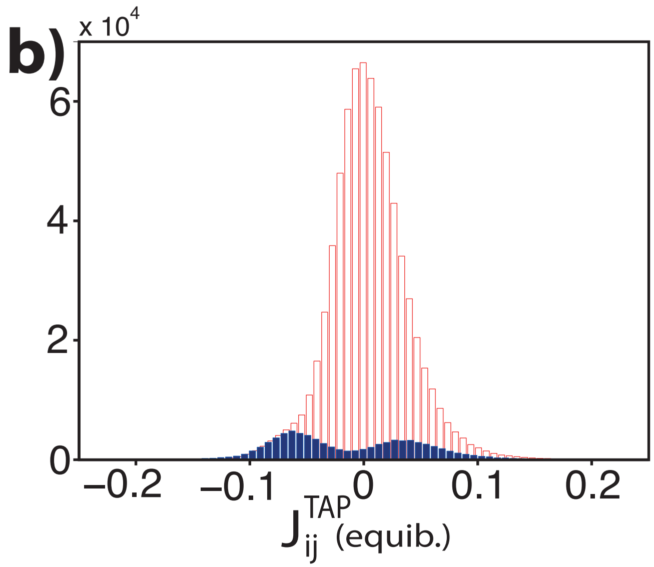


L=1000000

non-equilibrium



equilibrium



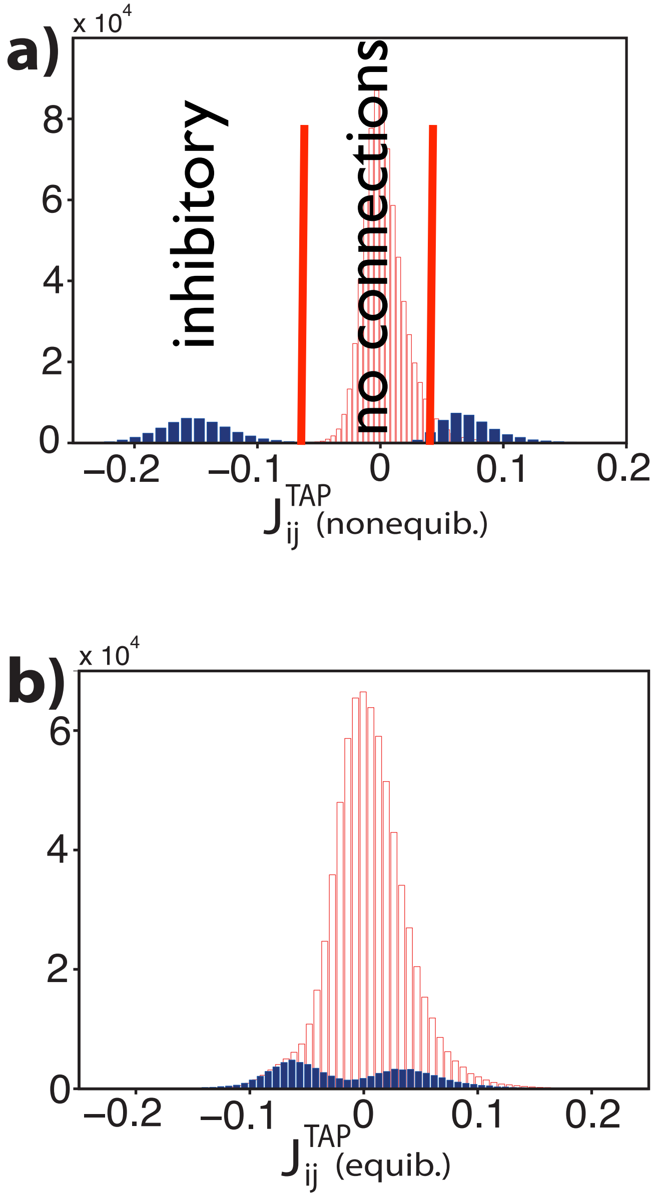
L=1000000

--- : synaptic connection present in original network

--- : synaptic connection absent in original network

non-
equilibrium

equilibrium



--- : synaptic connection present in original network

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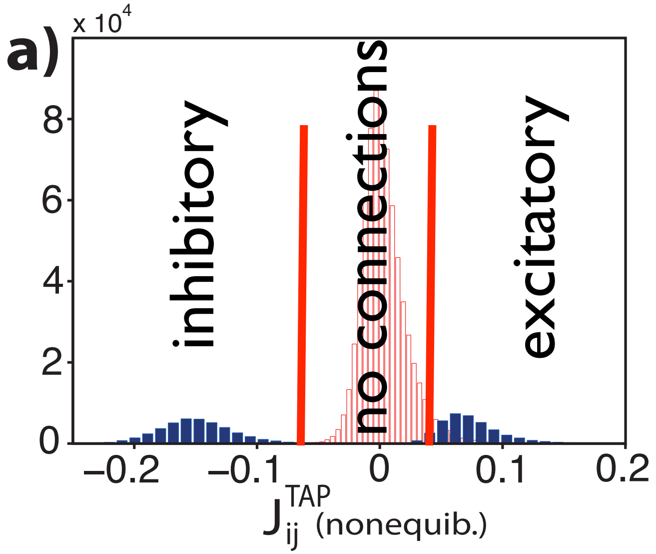
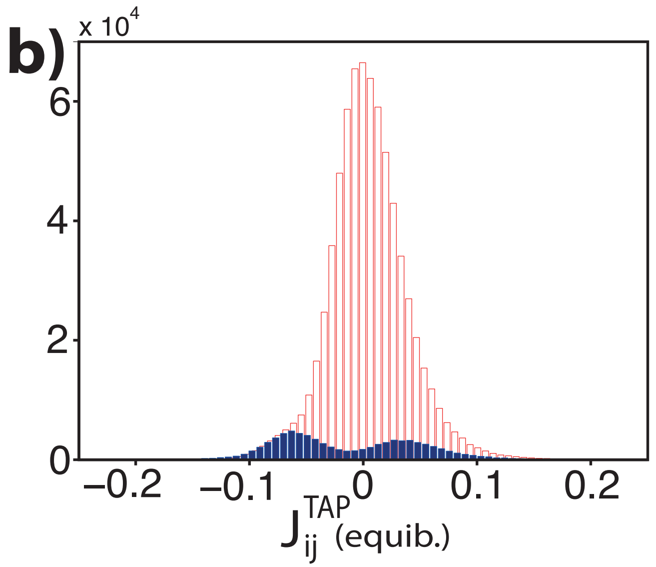
L=1000000

non-equilibrium



equilibrium



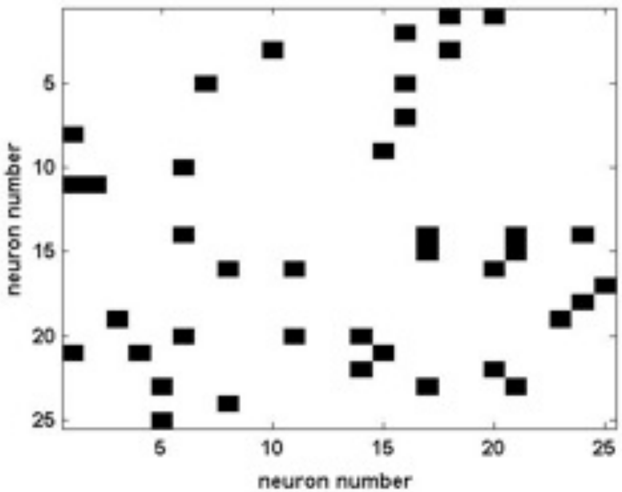
--- : synaptic connection present in original network

--- : synaptic connection absent in original network

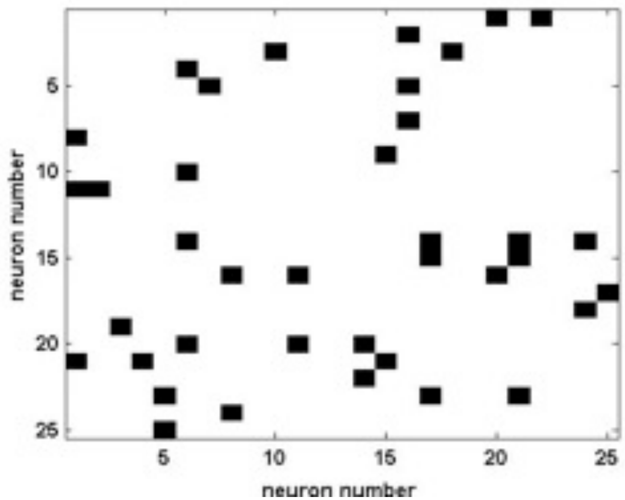
L=1000000

one example: 25 neurons

model connections:

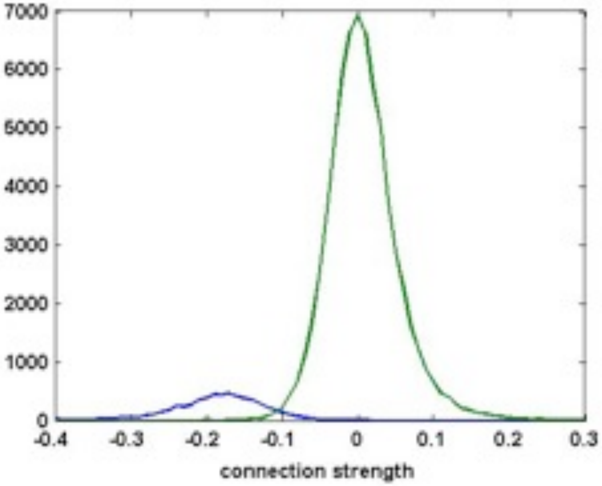


inferred connections:



noise/signal ratio

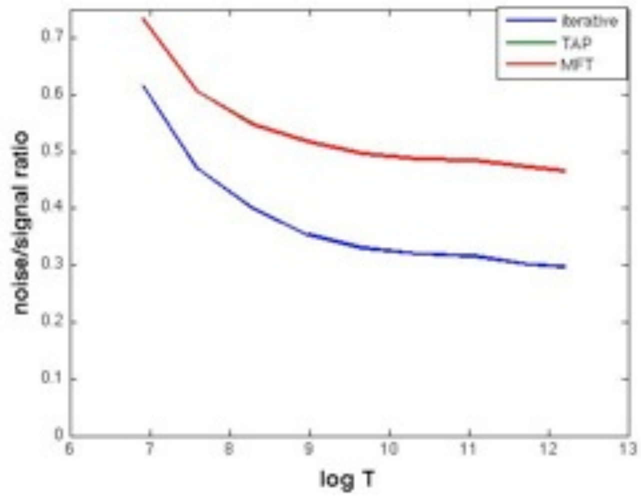
$$\mathrm{nsr} = \frac{\sigma_1 + \sigma_2}{\Delta J} = 0.5212$$



σ_1 σ_2

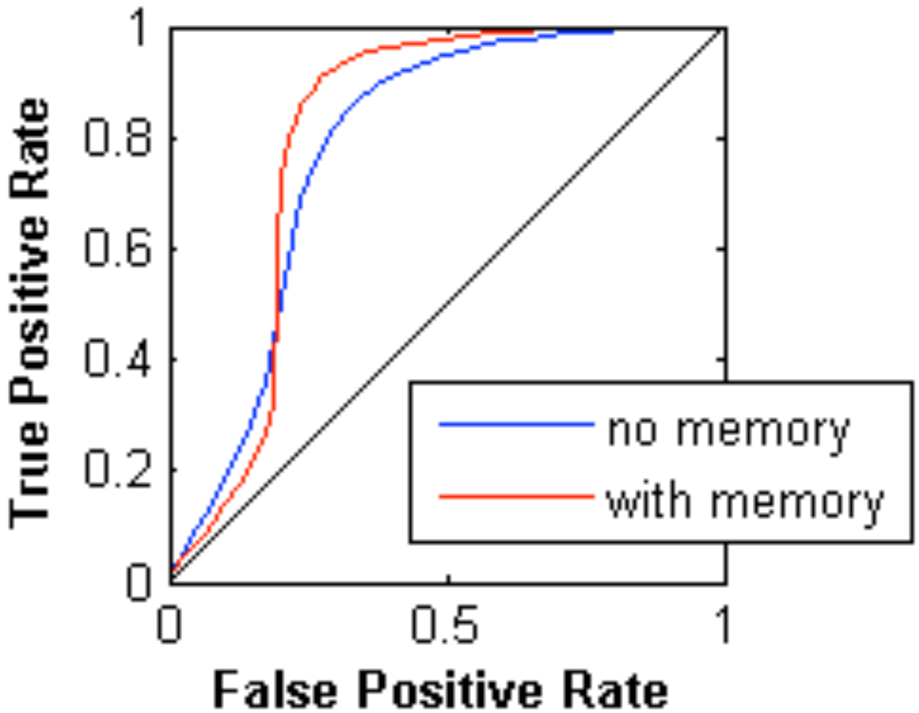
ΔJ

(95 inhibitory neurons)



(1000-200000 10-ms time bins)

you can also consider models with memory



work by Aree Witoelar

summary

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- we can also extend everything to the nonstationary regime.
- for simulated data, we can infer the connections.

notes

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- you can easily add l-1 and l-2 regularizer to the approximate inference methods.
- the issue of subsampling, i.e. observing only part of the system.
- relation to non-equilibrium FDTs (e.g. Prost et al PRL 2009)
- for asynchronous dynamics see Zeng et al, PRE 2011.
- full MF can be built for asymmetric SK model Mezard 2011

based on

Roudi Y., Hertz J., Mean field theory for non-equilibrium network reconstruction, PRL 2011

Roudi Y., Hertz J., Dynamical TAP equations for non-equilibrium Ising spin glasses, J Stat Mech 2011

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THE KAVLI FOUNDATION

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