## Online nonnegative matrix factorization for Markovian data

Deanna Needell

Joint work with Hanbaek Lyu, Laura Balzano and Chris Strohmeier. Partially supported by NSF DMS #2011140 and NSF BIGDATA #1740325.





Introduction

Algorithms for online NMF and their convergence

Applications of ONMF



Dr. Hanbaek Lyu (postdoc, UCLA → U. Wisconsin)



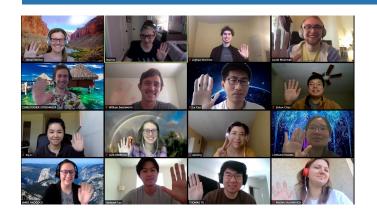
Prof. Laura Balzano (Univ Michigan)



Chris Strohmeier (PhD student, UCLA)



## Joint work with

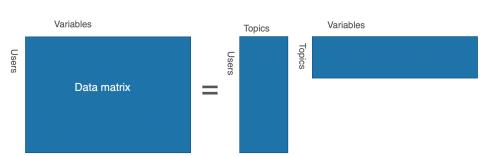




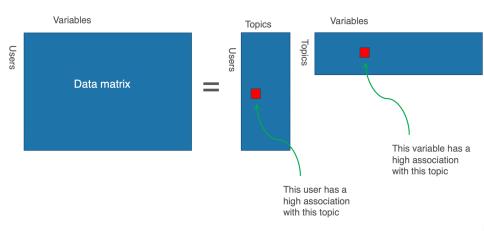


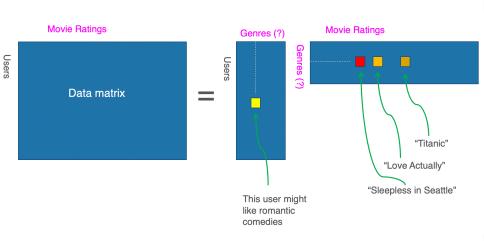


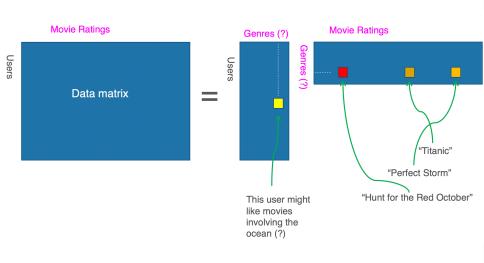
### Non-negative matrix factorization



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# (Semi)supervised NMF

- Incorporates label information to NMF
- $Y \in \mathbb{R}^{c \times n}$  = label matrix for c classes
- Find A, S,  $B \in \mathbb{R}^{c \times k}$  by

$$\min_{A \ge 0, S \ge 0, B \ge 0} \underbrace{\|(X - AS)\|_F^2}_{\text{Reconstruction Error}} + \lambda \underbrace{\|(Y - BS)\|_F^2}_{\text{Classification Error}}$$

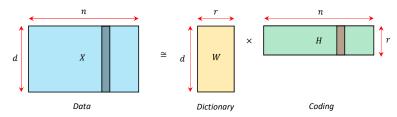


▶ The goal of **nonnegative matrix factorization** (NMF) is to factorize a data matrix  $X \in \mathbb{R}^{d \times n}_{\geq 0}$  into a pair of low-rank nonnegative matrices  $W \in \mathbb{R}^{d \times r}$  and  $H \in \mathbb{R}^{r \times n}$  by solving the following optimization problem

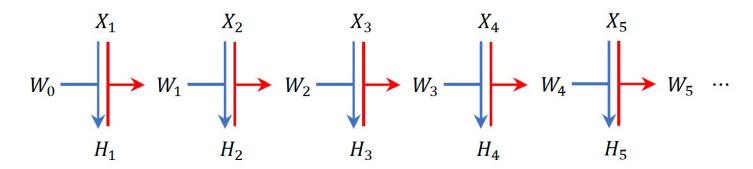
$$\inf_{W \in \mathbb{R}_{>0}^{d \times r}, \ H \in \mathbb{R}_{>0}^{r \times n}} ||X - WH||_F^2,$$

where  $||A||_F^2 = \sum_{i,j} A_{ij}^2$  denotes the matrix Frobenius norm.

▶ Data  $\approx$  Dictionary  $\times$  Coding



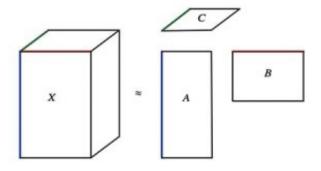
- Considers data that is streaming in over time
- Learns a factorization that is best (in expectation)
- Can be used for prediction in time series data
  - Uses "windows" across time to update factors and then predicts into a future window using one of the factors



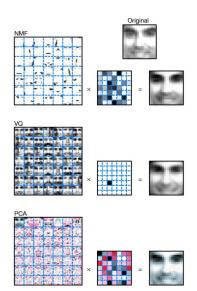


# Non-negative Tensor Factorization (NTF)

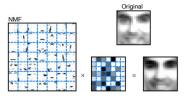
 Can be extended to tensors in a (nontrivial but) analogous way

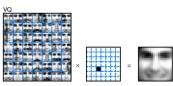


On the Topic of Topic Modeling

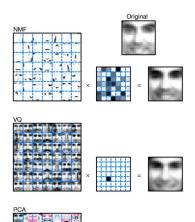


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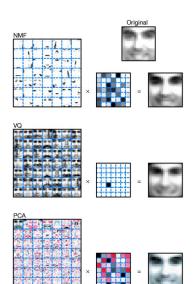




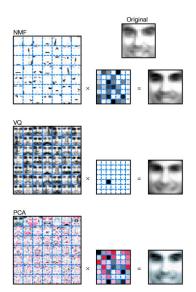
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- NMF was popularized by Lee and Seung in their Nature paper in 1999

#### Applications: Learning parts from images

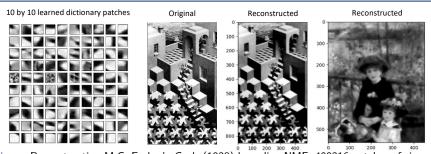
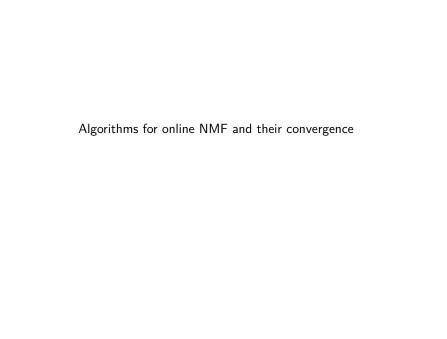
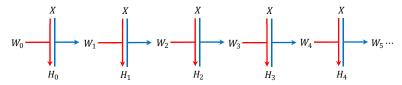


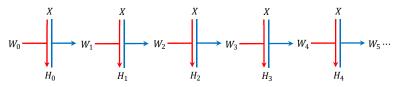
Figure: Reconstructing M.C. Escher's *Cycle* (1938) by online NMF. 400316 patches of size  $10 \times 10$  are extracted from the original image, and 100 dictionary patches (left) are learned by NMF. Original and reconstructed image using the learned dictionaries shown in the middle. The last shows the reconstructed image of Pierre-Auguste Renoir's *Two Sisters* (1882) (original image omitted) using the dictionary patches learned from Escher's *Cycle* in the left.



▶ In order to minimize  $||X - WH||_F$ , one can use block coordinate descent, by iteratively fixing W or H and minimizing the error w.r.t. the other factor



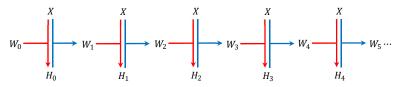
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▶ One of the most popular static NMF algorithm is the **Multiplicative Update** by Lee and Seung: Update all entries of *H* and *W* alternatively using the following update

$$H_{ij} \leftarrow H_{ij} \frac{[\boldsymbol{W}^T \boldsymbol{X}]_{ij}}{[\boldsymbol{W}^T \boldsymbol{W} \boldsymbol{X}]_{ij}}, \qquad W_{ij} \leftarrow W_{ij} \frac{[\boldsymbol{X} \boldsymbol{H}^T]_{ij}}{[\boldsymbol{X} \boldsymbol{H} \boldsymbol{H}^T]_{ij}}.$$

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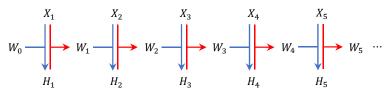
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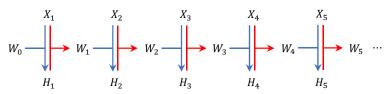
▶ It is known that the error  $||X - WH||_F^2$  is non-increasing under the above update, but there is no guarantee to converge to a stationary point.

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- ▶ The **online Non-negative Matrix Factorization** (ONMF) problem concerns a similar matrix factorization problem for a sequence of input matrices  $(x_T)_{t>0}$ .



▶ Suppose  $(X_t)_{t\geq 1}$  is an irreducible Markov chain on a sample space  $\Omega$  with unique stationary measure  $\pi$ . The goal of ONMF problem is to construct a sequence  $(W_t, H_t)_{t\geq 1}$  of dictionary  $W_t \in \mathbb{R}^{r \times d}$  and a coding  $H_t \in \mathbb{R}^{r \times n}$  such that (almost surely)

$$\|X_t - W_{t-1}H_t\|_F^2 \longrightarrow \inf_{W \in \mathbb{R}^{d \times t}, \ H \in \mathbb{R}^{r \times n}} \mathbb{E}_{X \sim \pi} \left[ \|X - WH\|_F^2 \right]$$

#### Naive ONMF algorithm minimizing empirical loss

Fix  $\lambda > 0$  and define the following the quadratic loss function

$$\ell(X, W) = \inf_{H \in \mathbb{R}^{r \times n}} ||X - WH||_F^2 + \lambda ||H||_1,$$

Define the expected loss and empirical loss functions

$$f(W) = \mathbb{E}_{X \sim \pi}[\ell(X, W)], \qquad f_t(W) = \frac{1}{t} \sum_{s=1}^t \ell(X_s, W)$$

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A naive solution to ONMF based on block optimization scheme:

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This requires to store all previous matrices and solve many optimization instances.

Online nonnegative matrix factorization for Markovian data

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- ▶ But we still need to store the entire history  $X_1, \dots, X_t$  and  $H_1, \dots, H_t$ . Do we?

▶ In fact, the approximate ONMF problem is equivalent to

$$\begin{aligned} \textit{Upon arrival of $X_t$:} & \begin{cases} H_t = \mathsf{argmin}_{H \in \mathbb{R}_{\geq 0}^{r \times n}} \|X_t - W_{t-1} H\|_F^2 + \lambda \|H\|_1 \\ A_t = t^{-1}((t-1)A_{t-1} + H_t H_t^T) \\ B_t = t^{-1}((t-1)B_{t-1} + H_t X_t^T) \\ W_t = \mathsf{argmin}_{W \in \mathcal{C} \subseteq \mathbb{R}_{\geq 0}^{d \times r}} \left( \mathsf{tr}(W A_t W^T) - 2 \mathsf{tr}(W B_t) \right), \end{cases}$$

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- ightharpoonup Computing  $W_t$  also requires solving only a single optimization instance

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### Theorem (Mairal, Bach, Ponce, and Sapiro '10)

Suppose  $(X_t)_{t\geq 0}$  are i.i.d. with common distribution  $\pi$ . Let  $(W_{t-1}, H_t)_{t\geq 1}$  be the optimal solution to the above ONMF algorithm.

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- (ii)  $\limsup_{t\to\infty} \|\nabla f(W_t)\|_{op} = 0$  almost surely.

### Convergence under Markovian dependence

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Suppose  $(X_t)_{t\geq 0}$  is an irreducible MC on a finite state space with unique stationary distribution  $\pi$ . Let  $(W_{t-1}, H_t)_{t\geq 1}$  be a solution to the above ONMF algorithm. Then the following hold.

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- (ii)  $f_t(W_t) \hat{f}_t(W_t) \to 0$  as  $t \to \infty$  almost surely.

### Convergence under Markovian dependence

$$\begin{aligned} \textit{Upon arrival of $X_t$:} & \begin{cases} H_t = \mathsf{argmin}_{H \in \mathbb{R}_{\geq 0}^{r \times n}} \|X_t - W_{t-1} H\|_F^2 + \lambda \|H\|_1 \\ A_t = t^{-1}((t-1)A_{t-1} + H_t H_t^T) \\ B_t = t^{-1}((t-1)B_{t-1} + H_t X_t^T) \\ W_t = \mathsf{argmin}_{W \in \mathcal{C} \subseteq \mathbb{R}_{\geq 0}^{d \times r}} \left( \mathsf{tr}(W A_t W^T) - 2 \mathsf{tr}(W B_t) \right), \end{cases}$$

 $f_t = \text{empirical loss}, \qquad \hat{f}_t = \text{surrogate loss}, \quad f = \text{expected loss}$ 

### Theorem (Balzano, Lyu, Needell '19+)

Suppose  $(X_t)_{t\geq 0}$  is an irreducible MC on a finite state space with unique stationary distribution  $\pi$ . Let  $(W_{t-1}, H_t)_{t\geq 1}$  be a solution to the above ONMF algorithm. Then the following hold.

- (i)  $\lim_{t\to\infty} \mathbb{E}[f_t(W_t)] = \lim_{t\to\infty} \mathbb{E}[\hat{f}_t(W_t)] < \infty.$
- (ii)  $f_t(W_t) \hat{f}_t(W_t) \to 0$  as  $t \to \infty$  almost surely.
- (iii)  $\limsup_{t\to\infty} \|\nabla f(W_t)\|_{op} = 0$  almost surely.

Applications of ONMF

## **MyLymeData**

- Lyme disease a vector-borne disease typically transmitted by tick or insect bite or blood-blood contact
  - Symptoms often mimic those of others, e.g. MS / ALS / Parkinsons / FMA ... and can become chronic
- o CDC estimates 300,000 new diagnoses each year
  - Likely a grandiose underestimate
- Poorly understood, poorly funded, poorly diagnosed, poorly treated





## **MyLymeData**

 MyLymeData launched Nov 2015 → ~14,000 patients registered

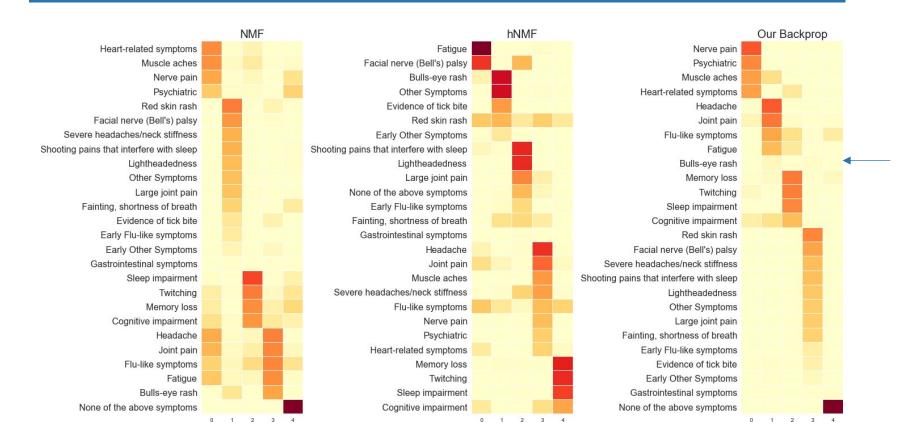
Type of data	# questions	Examples
Demographic	23	sex, age, birth country
Tick bite info	19	presence of EM rash, knowledge of bite, location, tick test results
Diagnostic info	34	# mis-diagnoses, time until diagnosis, # specialists
Early symptoms	11	rash, flu, neurologic, joint issues
Basic symptoms	13	(similar), with severity
Extended symptoms	54	(similar), with severity
Lab tests	21	CDC 2-tier, Western Blot, various blood markers
Co-infections	8	Babesia, Bartonella, Mycoplasma, Rickettsia
Treatment	129	effectiveness, type/style of antibiotics, duration, other treatments
Quality of life	54	sleep, ability to work, physical activity, improvements

Table 1: Patient supplied survey data description





## **Comparisons on Lyme data**

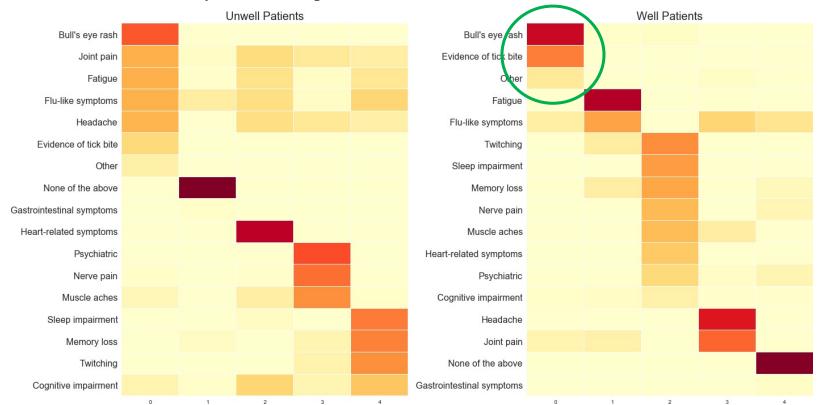


The hidden topics here may provide insight on how symptoms manifest themselves



# More Lyme data results

- Run our backpropagation separately on unwell and well datasets, then compare
- Notice the topics are very different!



On the Topic of Topic Modeling

#### Learning features from MCMC trajectories - Network Dictionary Learning

#### Mark Twain - Adventures of Huckleberry Finn

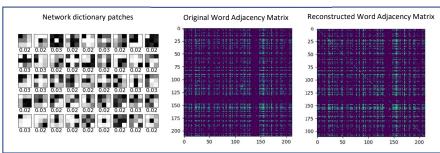


Figure: (Left) 45 learned 3 by 3 network dictionary patches from Glauber chain sampling from the Word Adjacency Matrix of "Mark Twain - Adventures of Huckleberry Finn". Black=1 and white = 0 with gray scale. (Middle) Heat map of the original Word Adjacency Matrix where blue = 0 and yellow = 1 (Right) the reconstruction.

#### Applications of ONMF

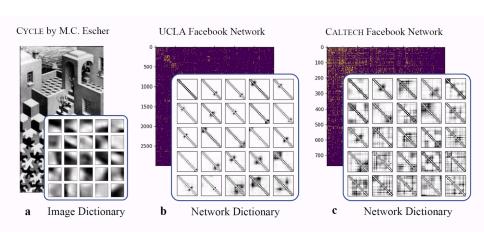


Figure: [6] (a) 25 latent shapes learned from an image by NMF. (b,c) 25 latent motifs for k = 21-node connected subgraphs learned from UCLA and CALTECH.

### ONMF for image reconstruction



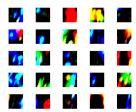




Fig. 7: Image Compression Via ONMF. (Top) uncompressed image of Leonid Afremov's famous painting "Rain's Rustle." (Middle) 25 of the 100 learned dictionary elements, reshaped from their vectorized form to color image patch form. (Bottom): Painting compressed using a dictionary of 100 vectorized 20 × 20 color image patches obtained from 30 data samples of ONMF, each consisting of 1000 randomly selected sample patches. We used an overlap length of 15 in the patch averaging for the construction of the compressed image.

#### ONMF for color restoration

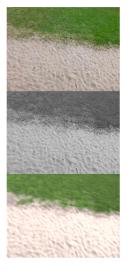
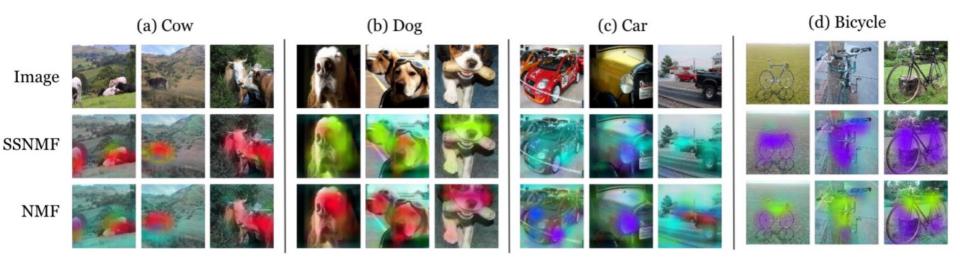




Fig. 8: Color Restoration. (First) Original image of grass and sand. (Second) Conversion of first image using matlab's default (linear) color to grayscale conversion function, rgb2gray. (Third) Restored color image, obtained by applying our method to the second (grayscale) image using the dictionary below. (Fourth) The first row displays the grass dictionary, the second row displays the sand dictionary. Each dictionary contains five 10 x 10 color image patches. These were trained on our ONMF with 20 batches of 1000 randomly selected sample patches each. We used maximal patch overlap in the restoration process.



# (O)NMF for image co-segmentation



### ONMF for video reconstruction

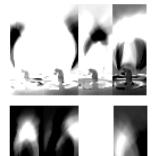


Fig. 4: Candle Video Dictionaries. The first dictionary consists of four elements and was trained by an alternating least squares-based, offline NMF, the second dictionary below was trained using ONMF, where each time frame of the video represented a new data point.

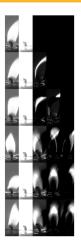


Fig. 5: Candle video and learned dictionary at various time frames (time goes from top to bottom). The left column corresponds to the actual video frame. The remaining four columns each correspond to a particular dictionary element. The six correspond to different time frames, 1, 5, 7, 15, 35, and 75

### ONMF for video denoising

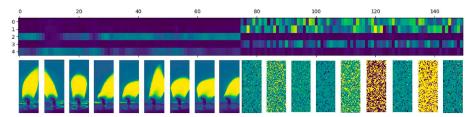


Fig. 6: Learning time evolution dictionary from a video frame using NMF. The first and last 75 frames of the video are from a candle video and white noise, respectively, as shown below. By an approximate factorization of shape [time x space] = [time  $x \le 1$  [5 x space], we learn  $150 \times 5$  dictionary matrix, whose columns give an approximate basis for the time evolution of each pixel of the video frame. The learned time evolution dictionaries detect the planeted 'phase transition' between frames 75 and 76.

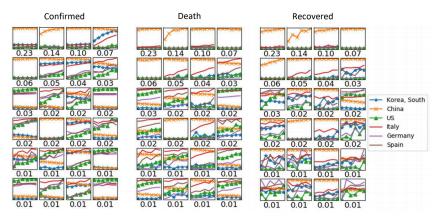


Fig. 2. 24 Joint dictionary atoms of 6-day evolution patterns of new daily cases (confirmed/death/recovered) in six countries (S. Korea, China, US, Italy, Germany, and France). Each dictionary atom is a 6 \* 6 \* 3 = 108 dimensional vector corresponding to time \*country\* case type. The corresponding importance metric is shown below each atom. 50 atoms are learned and the figure shows top 24 with the highest importance metric.

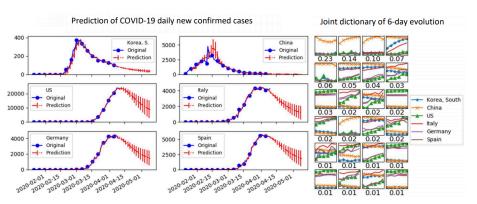


Fig. 3. Joint dictionary learning and prediction for the time-series of new daily cases (confirmed/death/recovered) in six countries (S. Korea, China, US, Italy, Germany, and France). After joint dictionary atoms are learned by minibatch learning, they are further adapted to the time-series data by concurrent online learning and predictions. (Right) Joint dictionary atoms of 6-day evolution patterns of new confirmed cases. The corresponding importance metric is shown below each atom. (Left) Plot of the original and predicted daily new confirmed cases of the six countries. The errorbar in the red plot shows standard deviation of 1000 trials.

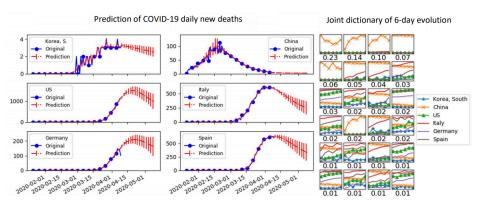


Fig. 4. Joint dictionary learning and prediction for the time-series of new daily cases (confirmed/death/recovered) in six countries (S. Korea, China, US, Italy, Germany, and France). After dictionary atoms representing fundamental joint time-series patterns are obtained by minibatch learning, they are further adapted to the time-series data by online learning while making predictions. (Right) Joint dictionary atoms of 6-day evolution patterns of new death cases. The corresponding importance metric is shown below each atom. (Left) The plot of the original and predicted daily new death cases of the six countries. The error bar in the red plot shows the standard deviation of 1000 trials.

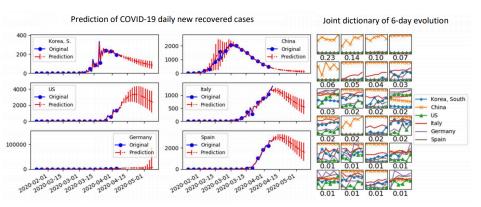


Fig. 5. Joint dictionary learning and prediction for the time-series of new daily cases (confirmed/death/recovered) in six countries (S. Korea, China, US, Italy, Germany, and France). After joint dictionary atoms are learned by minibatch learning, they are further adapted to the time-series by online learning while making predictions. (Right) Joint dictionary atoms of 6-day evolution patterns of new recovered cases. The corresponding importance metric is shown below each atom. (Left) The plot of the original and predicted daily new recovered cases of the six countries. The errorbar in the red plot shows the standard deviation of 1000 trials.

### Extension to Online NN Tensor Factorization (ONTF)

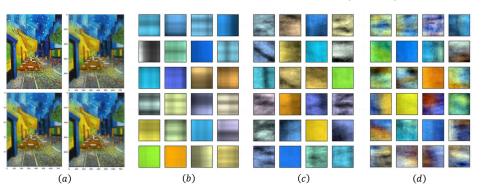
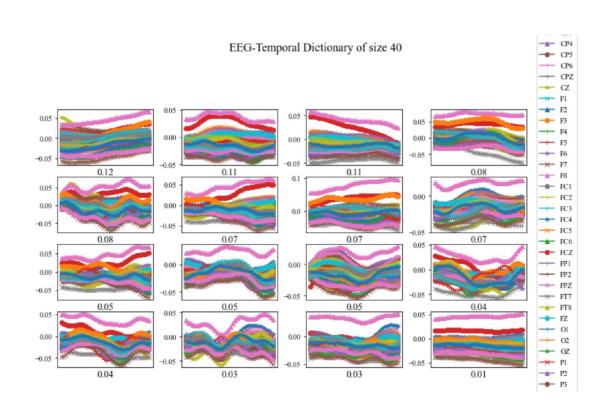


FIGURE 3. Learning 24 CP-dictionary patches by Online CPDL: (a) original (top left) and reconstructed images (top right from (b), bottom left from (c), and bottom right from (d)), (b) dictionary learned by Online CPDL, (c) dictionary learned by vectorizing the spatial modes and applying Online CPDL to resulting tensor then reshaping, (d) dictionary learned using online CPDL on fully vectorized image patch data.

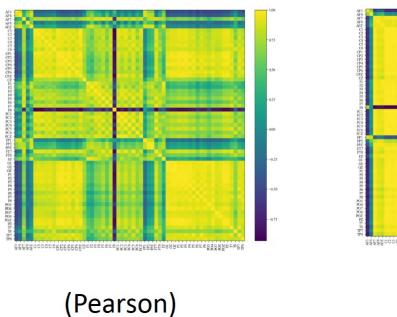


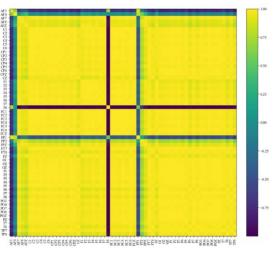
## ONMF on EEG node correlations (UCI EEG Alcoholism data, 64 electrodes)





## ONMF on EEG data (node correlations)

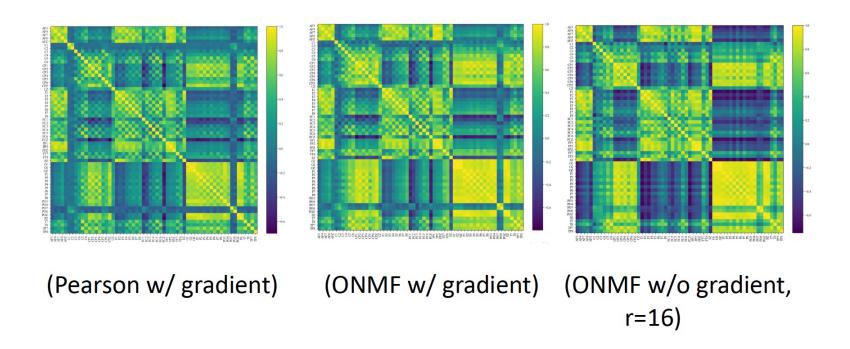




(ONMF)



## ONMF on EEG data (node correlations)



### ONTF to learn activation patterns in mouse cortex

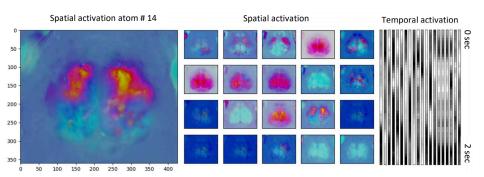


FIGURE 4. Learning 20 CP-dictionary patches from video frames on brain activity across the mouse cortex.

### ONTF to learn weather patterns

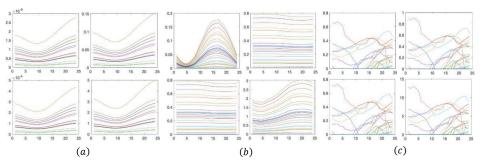


FIGURE 5. Display of one atom from three different dictionaries of 25 atoms which were obtained from Online CPDL on weather data: (a) no reshaping, (b) data which was reshaped to  $36 \times (24 \times 4)$ , and (c) data which was reshaped to  $(36 \times 24) \times 4$ .

#### Learning features from MCMC trajectories - Ising model

► The two dimensional Ising model (1920) is one of the most well-known spin systems in the physics literature, which models ferromagnetism.





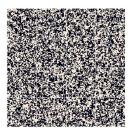


Figure: MCMC simulation of Ising model on 200 by 200 square lattice at temperature T=0.5 (left), T=2.26 (middle), and T=5 (right).

#### Learning features from MCMC trajectories - Ising model

- ▶ The two dimensional Ising model (1920) is one of the most well-known spin systems in the physics literature, which models ferromagnetism.
- ▶ For each temperature parameter T > 0, Define a probability distribution  $\pi$  on the set  $\{-1,1\}^{\mathbb{Z}^2}$  of spin configurations by

$$\pi_{\mathcal{T}}(\mathbf{x}) \propto \exp\left(-rac{1}{T}\sum_{i\sim j}\mathbf{x}(i)\mathbf{x}(j)
ight).$$





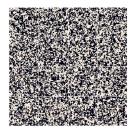


Figure: MCMC simulation of Ising model on 200 by 200 square lattice at temperature T=0.5 (left), T=2.26 (middle), and T=5 (right).

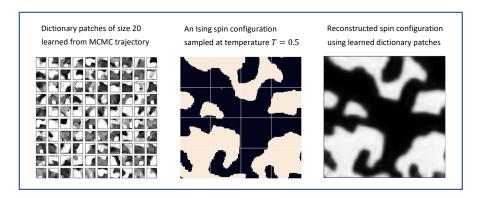
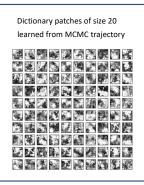
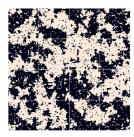


Figure: (Left) 100 learned dictionary patches from a MCMC Gibbs sampler for the Ising model on  $200 \times 200$  square lattice at a subcritical temperature (T=0.5). (Middle) A sampled spin configuration at T=0.5. (Right) Reconstruction of the original spin configuration in the middle using the dictionary patches on the left.



An Ising spin configuration sampled at temperature T=2.26



Reconstructed spin configuration using learned dictionary patches

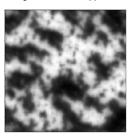


Figure: (Left) 100 learned dictionary patches from a MCMC Gibbs sampler for the Ising model on  $200 \times 200$  square lattice near the critical temperature (T=2.26). (Middle) A sampled spin configuration at T=2.26. (Right) Reconstruction of the original spin configuration in the middle using the dictionary patches on the left.

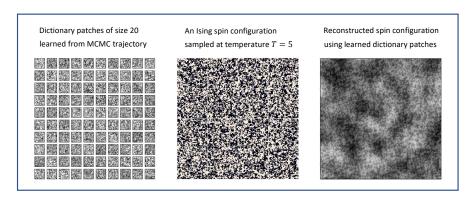
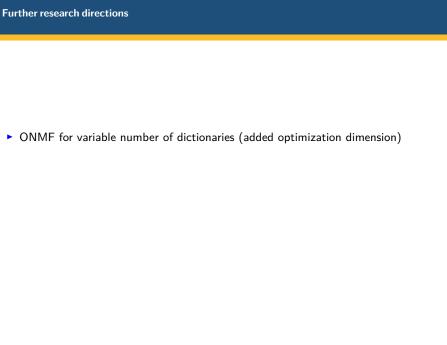


Figure: (Left) 100 learned dictionary patches from a MCMC Gibbs sampler for the Ising model on  $200 \times 200$  square lattice at a supercritical temperature (T=5). (Middle) A sampled spin configuration at T=5. (Right) Reconstruction of the original spin configuration in the middle using the dictionary patches on the left.



#### **Further research directions**

- ► ONMF for variable number of dictionaries (added optimization dimension)
- ▶ ONMF for non-stationary data matrices (what do we want to learn in this case?)

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- ONMF for variable number of dictionaries (added optimization dimension)
- ▶ ONMF for non-stationary data matrices (what do we want to learn in this case?)
- Dynamic topic modeling using ONMF
- Extension to online Tensor Factorization (no convergence result known even for the i.i.d. case)



# Thank you for listening!



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• math.ucla.edu/~deanna

# Thanks!

5. Proof of convergence

▶ Fix  $\lambda > 0$  and define the following the quadratic loss function

$$\ell(X, W) = \inf_{H \in \mathbb{R}^{r \times n}} ||X - WH||_F^2 + \lambda ||H||_1,$$

Define the expected loss and empirical loss functions

$$f(W) = \mathbb{E}_{X \sim \pi}[\ell(X, W)], \qquad f_t(W) = \frac{1}{t} \sum_{s=1}^{t} \ell(X_s, W)$$

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ONMF algorithm:

Upon arrival of 
$$X_t$$
: 
$$\begin{cases} H_t = \operatorname{argmin}_{H \in \mathbb{R}_{\geq 0}^{r \times n}} \|X_t - W_{t-1}H\|_F^2 + \lambda \|H\|_1 \\ W_t = \operatorname{argmin}_{W \in \mathcal{C}} \hat{f}_t(W), \end{cases}$$

where

$$\hat{f}_t(W) = \frac{1}{t} \sum_{s=1}^t (\|X_s - WH_s\|_F^2 + \lambda \|H_s\|_1).$$

▶ Fix  $\lambda > 0$  and define the following the **quadratic loss function** 

$$\ell(X, W) = \inf_{H \in \mathbb{R}^{r \times n}} ||X - WH||_F^2 + \lambda ||H||_1,$$

Define the expected loss and empirical loss functions

$$f(W) = \mathbb{E}_{X \sim \pi}[\ell(X, W)], \qquad f_t(W) = \frac{1}{t} \sum_{s=1}^{t} \ell(X_s, W)$$

ONMF algorithm:

Upon arrival of 
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$$\begin{cases} H_t = \operatorname{argmin}_{H \in \mathbb{R}_{\geq 0}^{r \times n}} \|X_t - W_{t-1}H\|_F^2 + \lambda \|H\|_1 \\ W_t = \operatorname{argmin}_{W \in \mathcal{C}} \hat{f}_t(W), \end{cases}$$

where

$$\hat{f}_t(W) = \frac{1}{t} \sum_{s=1}^t (\|X_s - WH_s\|_F^2 + \lambda \|H_s\|_1).$$

 $\blacktriangleright$  WTS:  $W_t$  converges to the set of critical points of the expected loss f

Let  $(W_{t-1}, H_t)_{t\geq 1}$  be a solution to the ONMF algorithm. Then for each  $t\geq 0$ , the followings hold almost surely:

(i) 
$$\hat{f}_{t+1}(W_{t+1}) - \hat{f}_t(W_t) \leq \frac{1}{t+1} (\ell(X_{t+1}, W_t) - f_t(W_t)).$$

(ii) 
$$0 \leq \frac{1}{t+1} \left( \hat{f}_t(W_t) - f_t(W_t) \right) \leq \frac{1}{t+1} \left( \ell(X_{t+1}, W_t) - f_t(W_t) \right) + \hat{f}_t(W_t) - \hat{f}_{t+1}(W_{t+1}).$$

▶ Recall that  $\hat{f}_t \ge f_t$  for all  $t \ge 0$ .

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- Recall that  $\hat{f}_t \geq f_t$  for all  $t \geq 0$ .
- Also note that  $\hat{f}_{t+1}(W_t) = \frac{1}{t+1} \left( t\hat{f}_t(W_t) + \ell(X_{t+1}, W_t) \right)$ .

Let  $(W_{t-1}, H_t)_{t\geq 1}$  be a solution to the ONMF algorithm. Then for each  $t\geq 0$ , the followings hold almost surely:

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$$\hat{f}_{t+1}(W_{t+1}) - \hat{f}_t(W_t) \leq \frac{1}{t+1} (\ell(X_{t+1}, W_t) - f_t(W_t)).$$

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- Also note that  $\hat{f}_{t+1}(W_t) = \frac{1}{t+1} \left( t\hat{f}_t(W_t) + \ell(X_{t+1}, W_t) \right)$ .

$$\begin{split} \hat{f}_{t+1}(W_{t+1}) - \hat{f}_{t}(W_{t}) &= \hat{f}_{t+1}(W_{t+1}) - \hat{f}_{t+1}(W_{t}) + \hat{f}_{t+1}(W_{t}) - \hat{f}_{t}(W_{t}) \\ &= \left[ \hat{f}_{t+1}(W_{t+1}) - \hat{f}_{t+1}(W_{t}) \right] + \frac{1}{t+1} \left( \ell(X_{t+1}, W_{t}) - f_{t}(W_{t}) \right) + \left[ \frac{f_{t}(W_{t}) - \hat{f}_{t}(W_{t})}{t+1} \right] \\ &\leq \frac{1}{t+1} \left( \ell(X_{t+1}, W_{t}) - f_{t}(W_{t}) \right). \end{split}$$

This shows (i). Using the second equality above and the fact that  $\hat{f}_{t+1}(W_{t+1}) \leq \hat{f}_{t+1}(W_t)$ , this also shows (ii).

Let  $(W_{t-1}, H_t)_{t\geq 1}$  be a solution to the ONMF algorithm. Then for each  $t\geq 0$ , the followings hold almost surely:

(i) 
$$\hat{f}_{t+1}(W_{t+1}) - \hat{f}_t(W_t) \leq \frac{1}{t+1} (\ell(X_{t+1}, W_t) - f_t(W_t)).$$

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## Sketch of main argument:

Let  $(W_{t-1}, H_t)_{t\geq 1}$  be a solution to the ONMF algorithm. Then for each  $t\geq 0$ , the followings hold almost surely:

(i) 
$$\hat{f}_{t+1}(W_{t+1}) - \hat{f}_t(W_t) \leq \frac{1}{t+1} (\ell(X_{t+1}, W_t) - f_t(W_t)).$$

(ii) 
$$0 \leq \frac{1}{t+1} \left( \hat{f}_t(W_t) - f_t(W_t) \right) \leq \frac{1}{t+1} \left( \ell(X_{t+1}, W_t) - f_t(W_t) \right) + \hat{f}_t(W_t) - \hat{f}_{t+1}(W_{t+1}).$$

#### Sketch of main argument:

▶ By bounding the sum of  $\frac{1}{t+1} (\ell(X_{t+1}, W_t) - f_t(W_t))$  in expectation, (i) will show that  $\mathbb{E}[\hat{f}_t(W_t)]$  converges.

Let  $(W_{t-1}, H_t)_{t\geq 1}$  be a solution to the ONMF algorithm. Then for each  $t\geq 0$ , the followings hold almost surely:

(i) 
$$\hat{f}_{t+1}(W_{t+1}) - \hat{f}_t(W_t) \leq \frac{1}{t+1} (\ell(X_{t+1}, W_t) - f_t(W_t)).$$

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$$0 \leq \frac{1}{t+1} \left( \hat{f}_t(W_t) - f_t(W_t) \right) \leq \frac{1}{t+1} \left( \ell(X_{t+1}, W_t) - f_t(W_t) \right) + \hat{f}_t(W_t) - \hat{f}_{t+1}(W_{t+1}).$$

## Sketch of main argument:

- ▶ By bounding the sum of  $\frac{1}{t+1} (\ell(X_{t+1}, W_t) f_t(W_t))$  in expectation, (i) will show that  $\mathbb{E}[\hat{f}_t(W_t)]$  converges.
- ▶ Then (ii) will show that  $\hat{f}_t(W_t) f_t(W_t) \to 0$  as  $t \to \infty$ .

Let  $(W_{t-1}, H_t)_{t\geq 1}$  be a solution to the ONMF algorithm. Then for each  $t\geq 0$ , the followings hold almost surely:

(i) 
$$\hat{f}_{t+1}(W_{t+1}) - \hat{f}_t(W_t) \leq \frac{1}{t+1} (\ell(X_{t+1}, W_t) - f_t(W_t)).$$

(ii) 
$$0 \leq \frac{1}{t+1} \left( \hat{f}_t(W_t) - f_t(W_t) \right) \leq \frac{1}{t+1} \left( \ell(X_{t+1}, W_t) - f_t(W_t) \right) + \hat{f}_t(W_t) - \hat{f}_{t+1}(W_{t+1}).$$

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- ▶ Then (ii) will show that  $\hat{f}_t(W_t) f_t(W_t) \to 0$  as  $t \to \infty$ .
- ▶ Since  $f_t \leq \hat{f}_t$  and every limit point of the sequence  $(W_t)_{t\geq 0}$  is a critical point of  $\hat{f}_{\infty}$ , this will show that every limit point of  $(W_t)_{t\geq 0}$  is also a critical point of f.

$$\mathbb{E}\left[\ell(X_{t+1}, W_t) - f_t(W_t) \,\middle|\, \mathcal{F}_t\right] = \mathbb{E}_{X \sim \pi}[\ell(X, W_t)] - f_t(W_t) \tag{1}$$

$$= f(W_t) - f_t(W_t) \le ||f - f_t||_{\infty}$$
 (2)

Suppose data matrices  $X_t$  are i.i.d. and let  $\mathcal{F}_t$  denote the information up to time t. Then

$$\mathbb{E}\left[\ell(X_{t+1}, W_t) - f_t(W_t) \,\middle|\, \mathcal{F}_t\right] = \mathbb{E}_{X \sim \pi}[\ell(X, W_t)] - f_t(W_t) \tag{1}$$

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- Averaging over  $\mathcal{F}_t$ , this gives

$$\mathbb{E}\left[\left(\mathbb{E}\left[\frac{\ell(X_{t+1}, W_t) - f_t(W_t)}{t+1} \middle| \mathcal{F}_t\right]\right)^+\right] \le t^{-3/2} \mathbb{E}[t^{1/2} || f - f_t ||_{\infty}] \tag{3}$$

$$= O(t^{-3/2}). (4)$$

#### Key estimate in the Markovian case

▶ If  $(X_t)_{t\geq 0}$  is Markovian, then  $\mathbb{E}[\ell(X_{t+1}, W) | \mathcal{F}_t]$  could be very different from  $f(W) = \mathbb{E}_{X \sim \pi}[\ell(X, W)]$ .

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- ▶ Instead, **condition on a distant past**  $\mathcal{F}_{t-N}$  and see how much the chain mixes to the stationary distribution during [t-N,t].

$$\begin{split} \mathbb{E}\left[\ell(X_{t+1}, W) \,\middle|\, \mathcal{F}_{t-N}\right] &= \sum_{\mathbf{x}' \in \Omega} \ell(\mathbf{x}', W) \, P^{N+1}(\mathbf{x}, \mathbf{x}') \\ &= \sum_{\mathbf{x}' \in \Omega} \ell(\mathbf{x}', W) \, \pi(\mathbf{x}') + \sum_{\mathbf{x}' \in \Omega} \ell(\mathbf{x}', W) (P^{N+1}(\mathbf{x}, \mathbf{x}') - \pi(\mathbf{x}')) \\ &\leq \sum_{\mathbf{x}' \in \Omega} \ell(\mathbf{x}', W) \, \pi(\mathbf{x}') + 2 \|\ell(\cdot, W)\|_{\infty} \|P^{N+1}(\mathbf{x}, \cdot) - \pi\|_{\mathcal{T}V} \\ &= \mathit{f}(W) + 2 \|\ell(\cdot, W)\|_{\infty} \|P^{N+1}(\mathbf{x}, \cdot) - \pi\|_{\mathcal{T}V}. \end{split}$$

Suppose (A1)'-(A2) and (M2). Fix  $W \in \mathcal{C}$ . Then for each  $t \geq 0$  and  $0 \leq N < t$ , conditional on the information  $\mathcal{F}_{t-N}$  up to time t-N,

$$\left| \mathbb{E} \left[ \ell(X_{t+1}, W) - f_t(W) \, \middle| \, \mathcal{F}_{t-N} \right] \right| \le |f(W) - f_{t-N}(W)| \tag{5}$$

$$+\frac{N}{t}\left(f_{t-N}(W)+\|\ell(\cdot,W)\|_{\infty}\right) \tag{6}$$

+ 
$$2\|\ell(\cdot, W)\|_{\infty} \sup_{\mathbf{x} \in \Omega} \|P^{N+1}(\mathbf{x}, \cdot) - \pi\|_{TV}.$$
 (7)

#### Lemma

Suppose (A1)'-(A2) and (M1) hold.

(i) Let  $(a_t)_{t\geq 0}$  be a sequence of non-decreasing non-negative integers such that  $a_t=o(t)$ . Then there exists absolute constants  $C_1,\,C_2,\,C_3>0$  such that for all sufficiently large  $t\geq 0$ ,

$$\begin{split} \mathbb{E}\left[\left|\mathbb{E}\left[\frac{\ell(X_{t+1},W_t) - f_t(W_t)}{t+1}\,\middle|\,\mathcal{F}_{t-a_t}\right]\right|\right] &\leq \frac{C_1}{t^{3/2}} + \frac{C_2}{t^2}a_t \\ &\qquad \qquad + \frac{C_3}{t}\sup_{\mathbf{x}\in\Omega}\lVert P^{a_t+1}(\mathbf{x},\cdot) - \pi\rVert_{TV}. \end{split}$$

#### Lemma

Suppose (A1)'-(A2) and (M1) hold.

(i) Let  $(a_t)_{t\geq 0}$  be a sequence of non-decreasing non-negative integers such that  $a_t=o(t)$ . Then there exists absolute constants  $C_1,\,C_2,\,C_3>0$  such that for all sufficiently large  $t\geq 0$ ,

$$\mathbb{E}\left[\left|\mathbb{E}\left[\frac{\ell(X_{t+1}, W_t) - f_t(W_t)}{t+1} \left| \mathcal{F}_{t-a_t}\right]\right|\right] \leq \frac{C_1}{t^{3/2}} + \frac{C_2}{t^2} a_t + \frac{C_3}{t} \sup_{\mathbf{x} \in \Omega} \|P^{a_t+1}(\mathbf{x}, \cdot) - \pi\|_{TV}.$$

(ii) Further assume that (M2) holds. Then we have

$$\sum_{t=0}^{\infty} \left( \mathbb{E}\left[ \hat{f}_{t+1}(W_{t+1}) - \hat{f}_{t}(W_{t}) \right] \right)^{+} \leq \sum_{t=0}^{\infty} \left| \mathbb{E}\left[ \frac{\ell(X_{t+1}, W_{t}) - f_{t}(W_{t})}{t+1} \right] \right| < \infty.$$

#### **Proof of Thm 1**

▶ Since  $\sum_{t=0}^{\infty} \left( \mathbb{E}\left[\hat{f}_{t+1}(W_{t+1}) - \hat{f}_{t}(W_{t})\right] \right)^{+} < \infty$ ,  $\mathbb{E}[\hat{f}_{t}(W_{t})]$  converges.

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- By the earlier inequalities and estimates,

$$\begin{split} \mathbb{E}\left[\sum_{t=0}^{\infty} \frac{\hat{f}_t(W_t) - f_t(W_t)}{t+1}\right] &= \sum_{t=0}^{\infty} \frac{\mathbb{E}[\hat{f}_t(W_t)] - \mathbb{E}[f_t(W_t)]}{t+1} \\ &\leq \sum_{t=0}^{\infty} \left| \frac{\mathbb{E}[\ell(X_{t+1}, W_t)] - f_t(W_t)]}{t+1} \right| \\ &- \sum_{t=0}^{\infty} \left( \mathbb{E}[\hat{f}_{t+1}(W_{t+1})] - \mathbb{E}[\hat{f}_t(W_t)] \right) \\ &< \infty. \end{split}$$

- ▶ Since  $\sum_{t=0}^{\infty} \left( \mathbb{E}\left[\hat{f}_{t+1}(W_{t+1}) \hat{f}_{t}(W_{t})\right] \right)^{+} < \infty$ ,  $\mathbb{E}[\hat{f}_{t}(W_{t})]$  converges.
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$$\mathbb{E}\left[\sum_{t=0}^{\infty} \frac{\hat{f}_t(W_t) - f_t(W_t)}{t+1}\right] = \sum_{t=0}^{\infty} \frac{\mathbb{E}[\hat{f}_t(W_t)] - \mathbb{E}[f_t(W_t)]}{t+1}$$

$$\leq \sum_{t=0}^{\infty} \left| \frac{\mathbb{E}[\ell(X_{t+1}, W_t)] - f_t(W_t)]}{t+1} \right|$$

$$-\sum_{t=0}^{\infty} \left( \mathbb{E}[\hat{f}_{t+1}(W_{t+1})] - \mathbb{E}[\hat{f}_t(W_t)] \right)$$

$$< \infty.$$

▶ Hence  $\sum_{t=0}^{\infty} \frac{\hat{f}_t(W_t) - f_t(W_t)}{t+1} < \infty$  a.s. This implies  $\hat{f}_t(W_t) - f_t(W_t) \to 0$  a.s. as  $t \to \infty$ .

- ▶ Since  $\sum_{t=0}^{\infty} \left( \mathbb{E}\left[\hat{f}_{t+1}(W_{t+1}) \hat{f}_{t}(W_{t})\right] \right)^{+} < \infty$ ,  $\mathbb{E}[\hat{f}_{t}(W_{t})]$  converges.
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- $\blacktriangleright \text{ Hence } \textstyle \sum_{t=0}^{\infty} \frac{\hat{f}_t(W_t) f_t(W_t)}{t+1} < \infty \text{ a.s. This implies } \hat{f}_t(W_t) f_t(W_t) \to 0 \text{ a.s. as } t \to \infty.$
- ▶ Since  $\hat{f}_t \ge f_t$  and  $\hat{f}_t(W_t) f_t(W_t) \to 0$  a.s., argue that  $W_t$  has to converge to the set of critical points of  $f = \lim_{t \to \infty} f_t$ .