

Bayesian Tensor Decomposition: Dynamics and Sparsity

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School of computing, The University of Utah For ZJU talk



Outline

- 1. Background
- 2. Tensor learning via Bayesian Inference
- 3. Dynamics in Tensor (ICML 2022 oral paper)
- 4. Sparsity in Tensor(UAI & ICML 2021 paper)



Tensor Data: Widely Used High-Order Data Structures to Represent Interactions of Multiple Objects/Entities



(user, movie, episode)



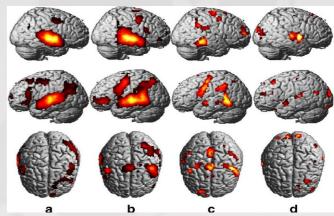
(location, region, time, climate)



(user, advertisement, page-section)



(user, location, message-type)



(subject, voxel, electrode)



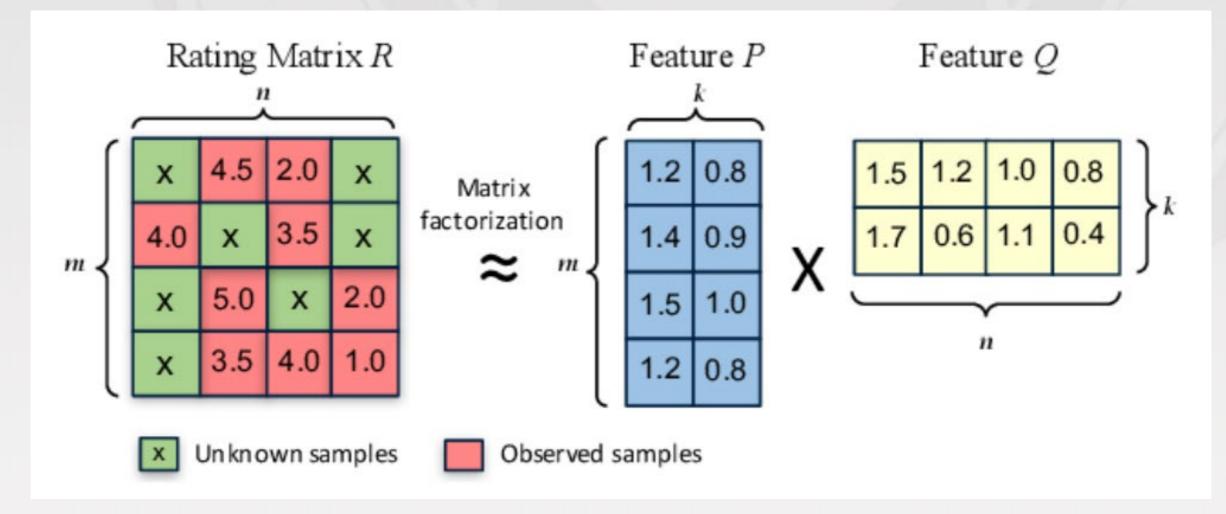
(patient, gene, condition)



Tensor Decomposition: estimate latent factors to reconstruct tensor with observed entries

• Simple case:

Collaborative Filtering (Matrix Factorization)



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• Simple case:

Collaborative Filtering (Matrix Factorization)

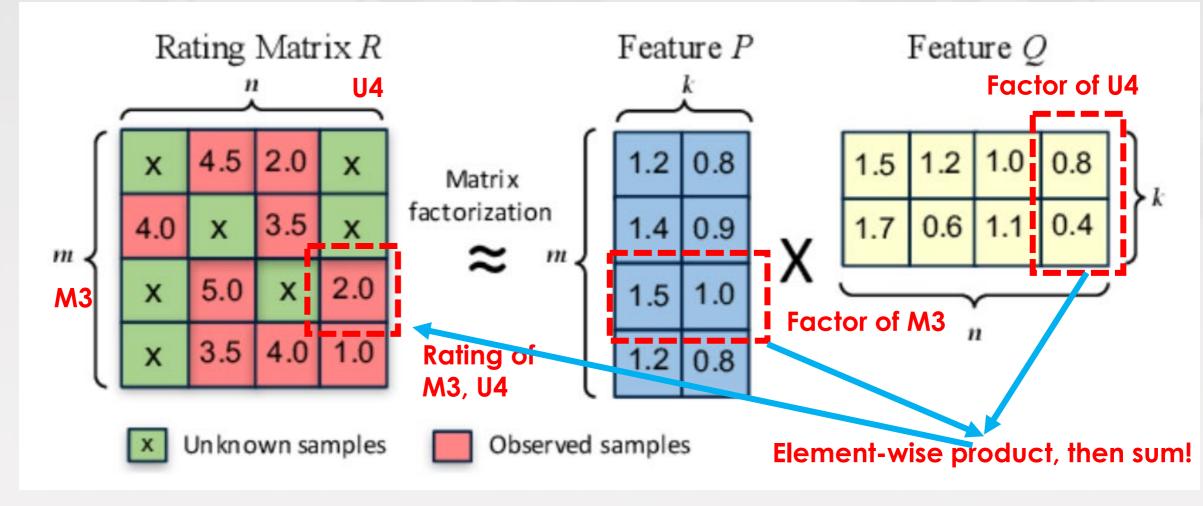


Image from https://www.slideshare.net/hontolab/matrix-factorization-192159058

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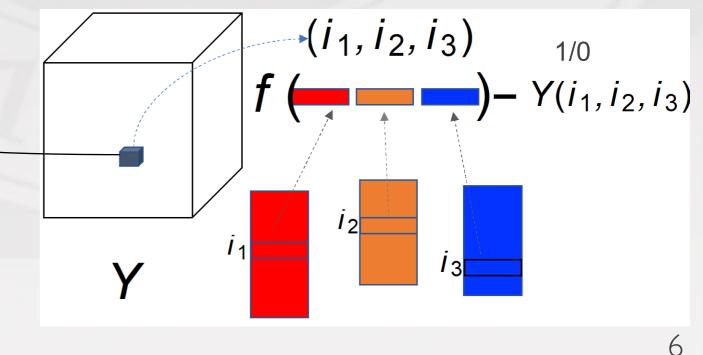
From matrix to tensor: **CP decomposition**

• Example of three-mode tensor:

$$\mathcal{X} \in \mathbb{R}^{I \times J \times K}, A \in \mathbb{R}^{I \times R}, B \in \mathbb{R}^{J \times R}, C \in \mathbb{R}^{K \times R}$$
$$x_{ijk} \approx \sum_{r=1}^{R} A_{ir} B_{jr} C_{kr} \text{ for } i = 1, \dots, I, j = 1, \dots, J, k = 1, \dots, K$$

Element-wise product, then sum! Interaction Records

user	item	page	purchase
100	25	35	1
23	21	56	0
100	25	35	1
32	33	46	0





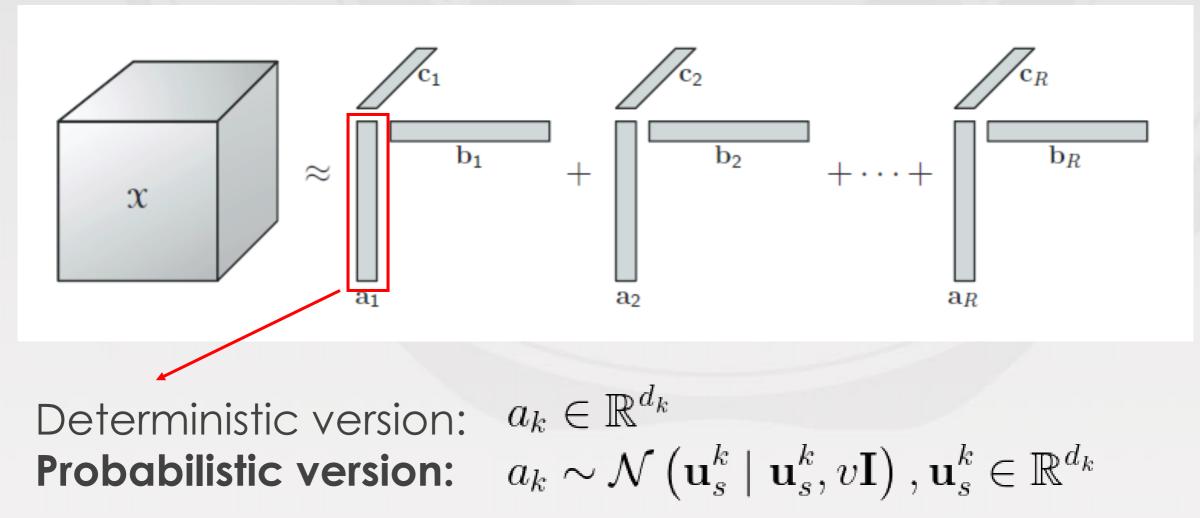
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- Make latent factor from variable to a distribution
- Turns Deterministic model -> Bayesian model

Uncertainty really counts!



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Bayesian version for CP decomposition,
the joint distribution is:

Observed data, factors, noise Prior of the noise
$$p(\{y_i\}_{i \in S} | \mathcal{U}, \tau) = Gam(\tau \mid a_0, b_0) \prod_{k=1}^{K} \prod_{s=1}^{d_k} \mathcal{N}(\mathbf{u}_s^k \mid \mathbf{m}_s^k, v\mathbf{I})$$

$$\prod_{i \in S} \mathcal{N}(y_i \mid \mathbf{1}^\top (\mathbf{u}_{i_1}^1 \circ \ldots \circ \mathbf{u}_{i_K}^K), \tau^{-1})$$

Gauss likelihood of the prediction

Final goal : Get the **exact posterior distribution :** $p(\mathcal{U}, \tau | \{y_{\mathbf{i}}\}_{\mathbf{i} \in S}) = \frac{p(\{y_{\mathbf{i}}\}_{\mathbf{i} \in S}, \mathcal{U}, \tau)}{p(\{y_{\mathbf{i}}\}_{\mathbf{i} \in S})}$

Distribution of data, Constant, we never know!!



- Exact posterior distribution p is always intractable
 Approximation it by a tractable distribution: q
- $p\left(\mathcal{U},\tau \mid \{y_{\mathbf{i}}\}_{\mathbf{i}\in S}\right) \approx q(\mathcal{U},\tau) = q(\tau) \prod_{k=1}^{K} \prod_{s=1}^{d_{k}} q\left(\mathbf{u}_{s}^{k}\right)$ $= \operatorname{Gamma}(\tau \mid a^{\star}, b^{\star}) \prod_{k=1}^{K} \prod_{s=1}^{d_{k}} \mathcal{N}\left(\mathbf{u}_{s}^{k} \mid \boldsymbol{\mu}_{s}^{k \star}, \boldsymbol{\Sigma}_{s}^{k \star}\right)$

Parameters needed to be optimized to make the approximation accurate !!

Become a problem of distribution match!



• Key point in Bayesian machine learning

$$p\left(\{y_{\mathbf{i}}\}_{\mathbf{i}\in S}, \mathcal{U}, \tau\right) = \operatorname{Gam}\left(\tau \mid a_{0}, b_{0}\right) \prod_{k=1}^{K} \prod_{s=1}^{d_{k}} \mathcal{N}\left(\mathbf{u}_{s}^{k} \mid \mathbf{m}_{s}^{k}, v\mathbf{I}\right)$$
$$\prod_{\mathbf{i}\in S} \mathcal{N}\left(y_{\mathbf{i}} \mid f\left(\mathbf{u}_{i_{1}}^{1}, \dots, \mathbf{u}_{i_{K}}^{K}\right), \tau^{-1}\right)$$

 $p(\mathcal{U}, \tau | \{y_{\mathbf{i}}\}_{\mathbf{i} \in S}) \approx q(\mathcal{U}, \tau) = q(\tau) \prod_{k=1}^{K} \prod_{s=1}^{d_k} q(\mathbf{u}_s^k)$

$$= \operatorname{Gamma}(\tau \mid a^{\star}, b^{\star}) \prod_{k=1}^{K} \prod_{s=1}^{d_{k}} \mathcal{N}\left(\mathbf{u}_{s}^{k} \mid \boldsymbol{\mu}_{s}^{k} \star, \boldsymbol{\Sigma}_{s}^{k} \star\right)$$

- Complete toolbox, but no silver bullet.
- Depend on the model f picked for the likelihood



Most-frequently used tool: Variational inference(VI): minimize the KL divergence of two distributions

$$\mathcal{L} = \int q^*(\mathcal{U}, \tau) \log \frac{p\left(\{y_i\}_{i \in S_t} \mid \mathcal{U}, \tau\right) q(\mathcal{U}, \tau)}{q^*(\mathcal{U}, \tau)} \mathrm{d}\mathcal{U} \mathrm{d}\tau$$

- Expectation propagation(EP): moment match when L(reverse order) has closed form solution
- Assumed density filtering(ADF): moment match when having tractable normalization term
- Reparameterization trick (SVI):
 Probabilistic version SGD when L is totally intractable
 ... (sampling based methods)



Series of work from our group under such architecture.

Short Names	Likelihood Model & Prior	Inference Method	Publication
POST[1]	CP decomposition/multi- linear	EP	ICDM 2018
POND[2]	Neural-kernel Gaussian process	SVI	ICDM 2020
SBTD[3]	Bayesian neural network + Sparse	ADF (Streaming)	ICML 2021
BASS[4]	Tucker decomposition + Sparse	ADF (Streaming)	UAI 2021
BCTT[5]	Tucker decomposition + Dynamics	CEP + KF/RTS	ICML 2022

[1]Du, Yishuai, et al. "Probabilistic streaming tensor decomposition." 2018 IEEE International Conference on Data Mining (ICDM). IEEE, 2018.
 [2]Conor Tillinghast, Shikai Fang, Kai Zheng, and Shandian Zhe, "Probabilistic Neural-Kernel Tensor Decomposition", IEEE International Conference on Data Mining (ICDM), 2020.

[3] Fang, Shikai, et al. "Streaming Probabilistic Deep Tensor Factorization." The Thirty-eighth International Conference on Machine Learning (ICML), 2021

[4] Fang, Shikai, et al. "Bayesian Streaming Sparse Tucker decomposition." Conference on Uncertainty in Artificial Intelligence. UAI, 2021.
 [5] Fang, Shikai, et al. "Bayesian Continues-Time Tucker Decomposition." The Thirty-ninth International Conference on Machine Learning (ICML), 2022



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Shikai Fang, Akil Narayan, Robert M. Kirby, and Shandian Zhe, "Bayesian Continuous-Time Tucker Decomposition" (Oral), The 39th International Conference on Machine Learning (ICML), 2022



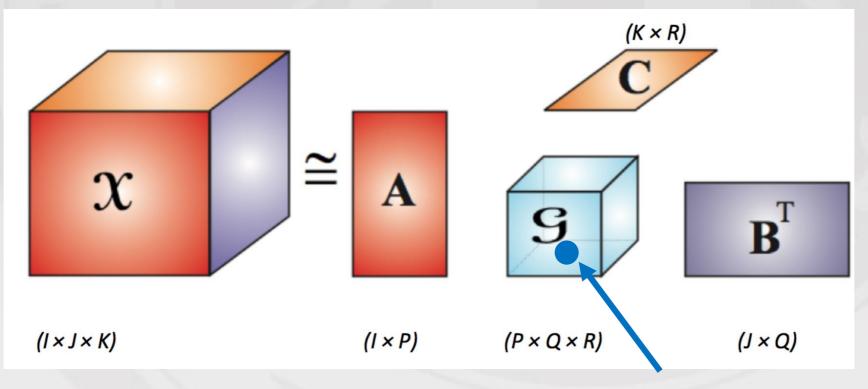
Tucker Decomposition

• 2-D matrix => N-D tensor

• Element-wise interaction => all possible interactions



Tucker Decomposition



One interaction weight

Element-wise form for a K-mode tensor Y:

Image from https://iksinc.online/2018/05/02/understanding-tensors-and-tensor-decompositions-part-3/.



Challenge: Temporal info in Tensor

What about each entry is time-dependent?

Straightforward Solution:

Drop time or

 $X_{ijk}(t)$

 Augment tensor with time-step mode

$(I \times J \times K)$

Problem:

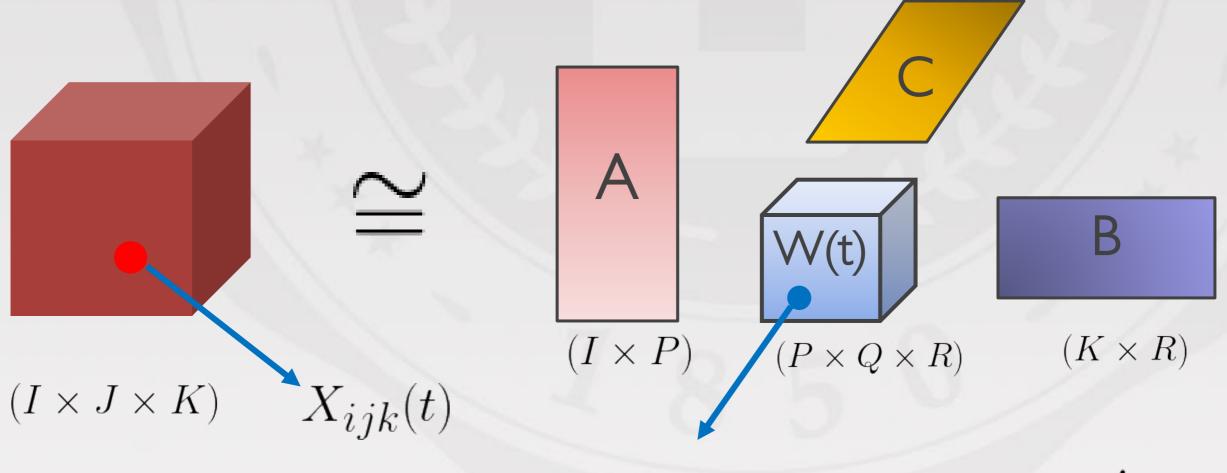
- 1. Too Sparse
- 2. Ignore the temporary continuity

 $(I \times J \times K \times T)$

t2



Our Solution: Modeling <u>Dynamic Tucker Core</u> by <u>Temporal Gaussian Processes</u>

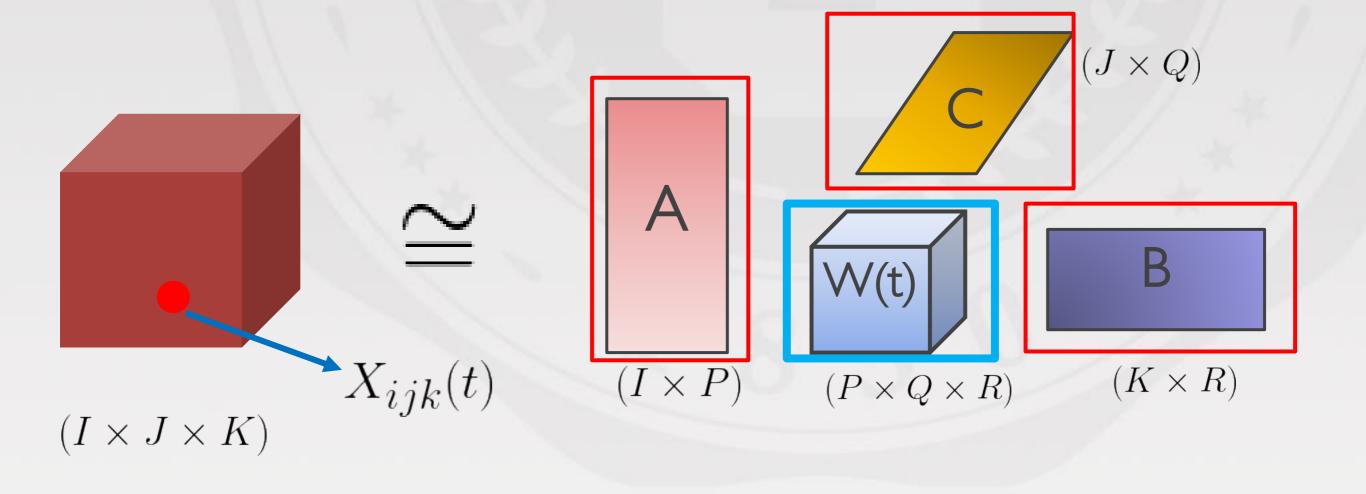


 $W_{pqr}(t) \sim GP(0, k(t, t'))$

 $(J \times Q)$



High-level Motivation: <u>Decouple</u> the representation learning of factors and the capture of dynamic pattern





Joint Probability:

$$\begin{array}{l} p\left(\mathcal{U}, \left\{\mathbf{w}_{\mathbf{r}}\right\}_{\mathbf{r}}, \tau, \mathbf{y}\right) = \\ \operatorname{Gam}\left(\tau \mid b_{0}, c_{0}\right) \prod_{k=1}^{K} \prod_{j=1}^{d_{k}} \mathcal{N}\left(\mathbf{u}_{j}^{k} \mid \mathbf{0}, \mathbf{I}\right) \times \prod_{\mathbf{r}=(1,...,1)}^{R_{1},...,R_{K}} \mathcal{N}\left(\mathbf{w}_{\mathbf{r}} \mid \mathbf{0}, \mathbf{K}_{\mathbf{r}}\right) \times \end{array}$$

Priors of factors and noise

Temporal GPs on Tucker Core

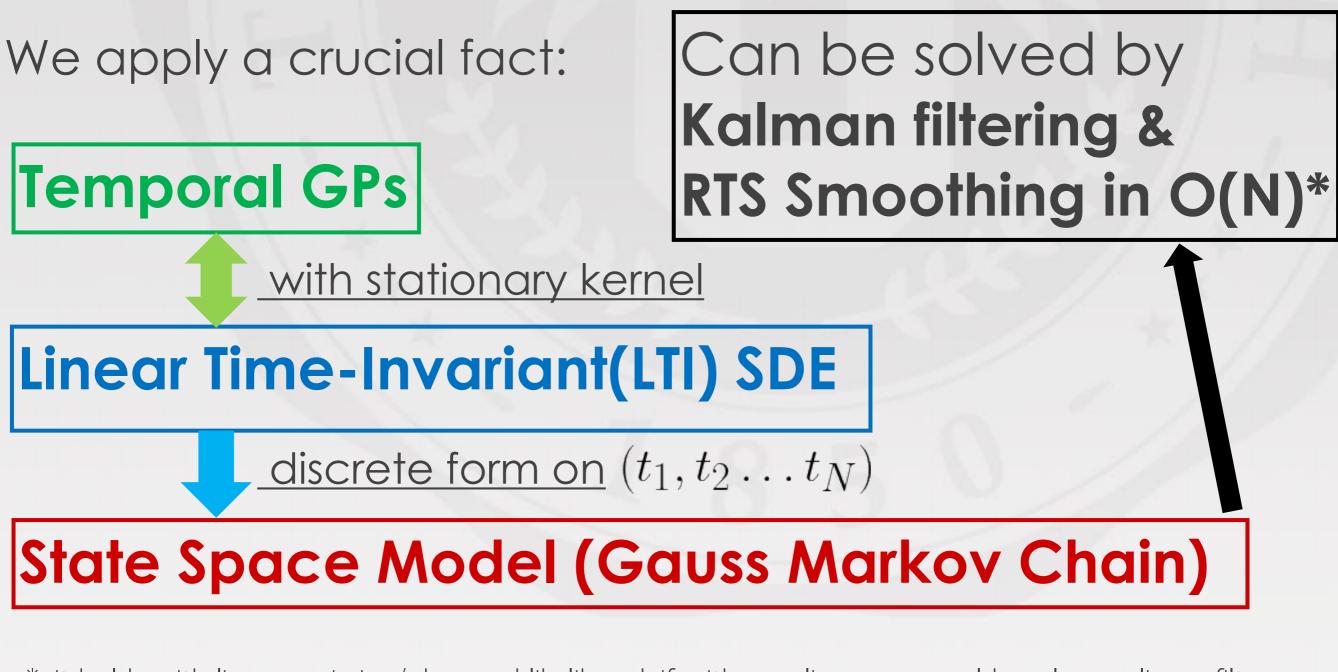
$$\prod_{n=1}^{N} \mathcal{N}\left(y_{n} \mid \operatorname{vec}\left(\mathcal{W}\left(t_{n}\right)\right)^{\top}\left(\mathbf{u}_{i_{n_{1}}}^{1} \otimes \ldots \otimes \mathbf{u}_{i_{n_{K}}}^{K}\right), \tau^{-1}\right)$$

Gaussian Likelihood

Computational challenge: O(N^3) cost of full GPs



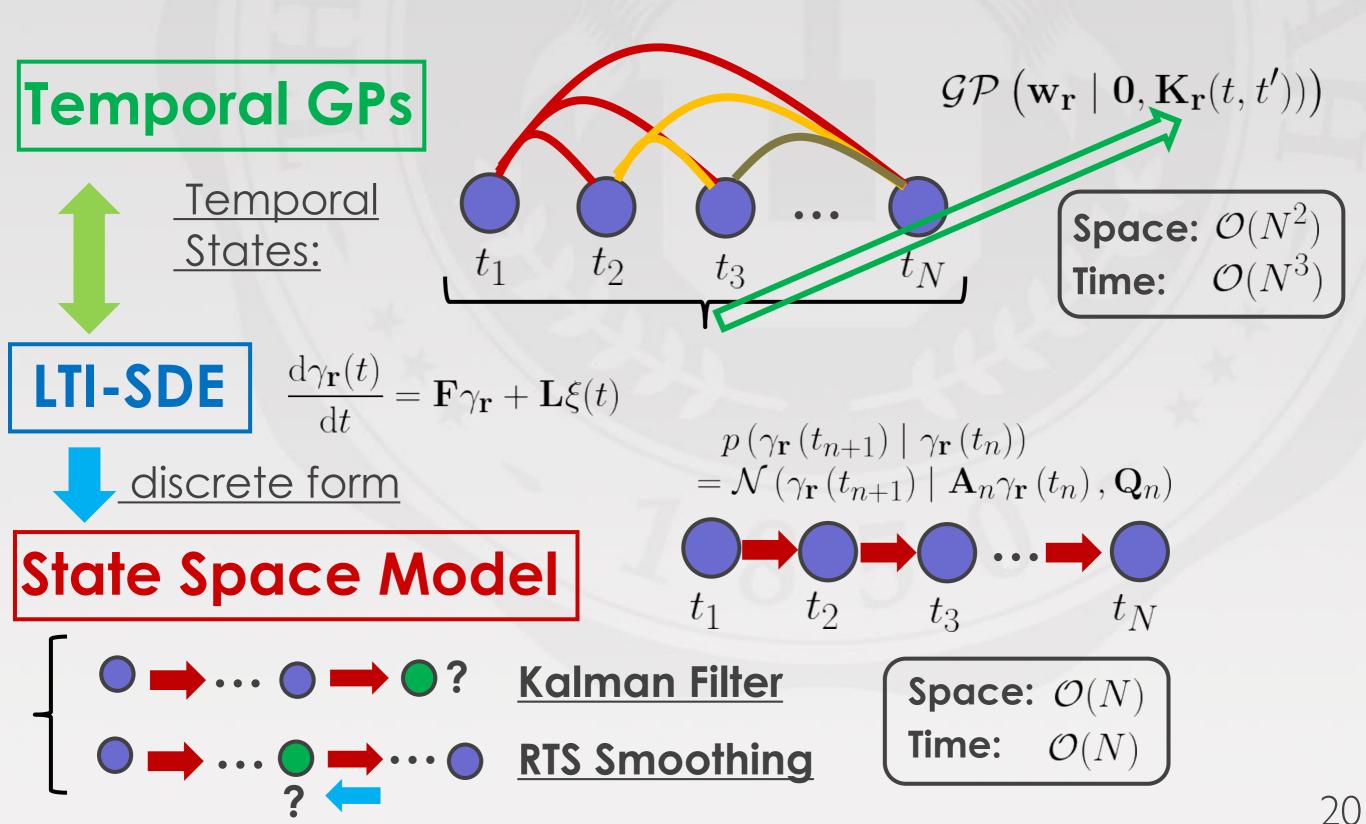
To avoid low-rank/sparse approx. (low quality), but enjoy linear-cost inference of full GPs,

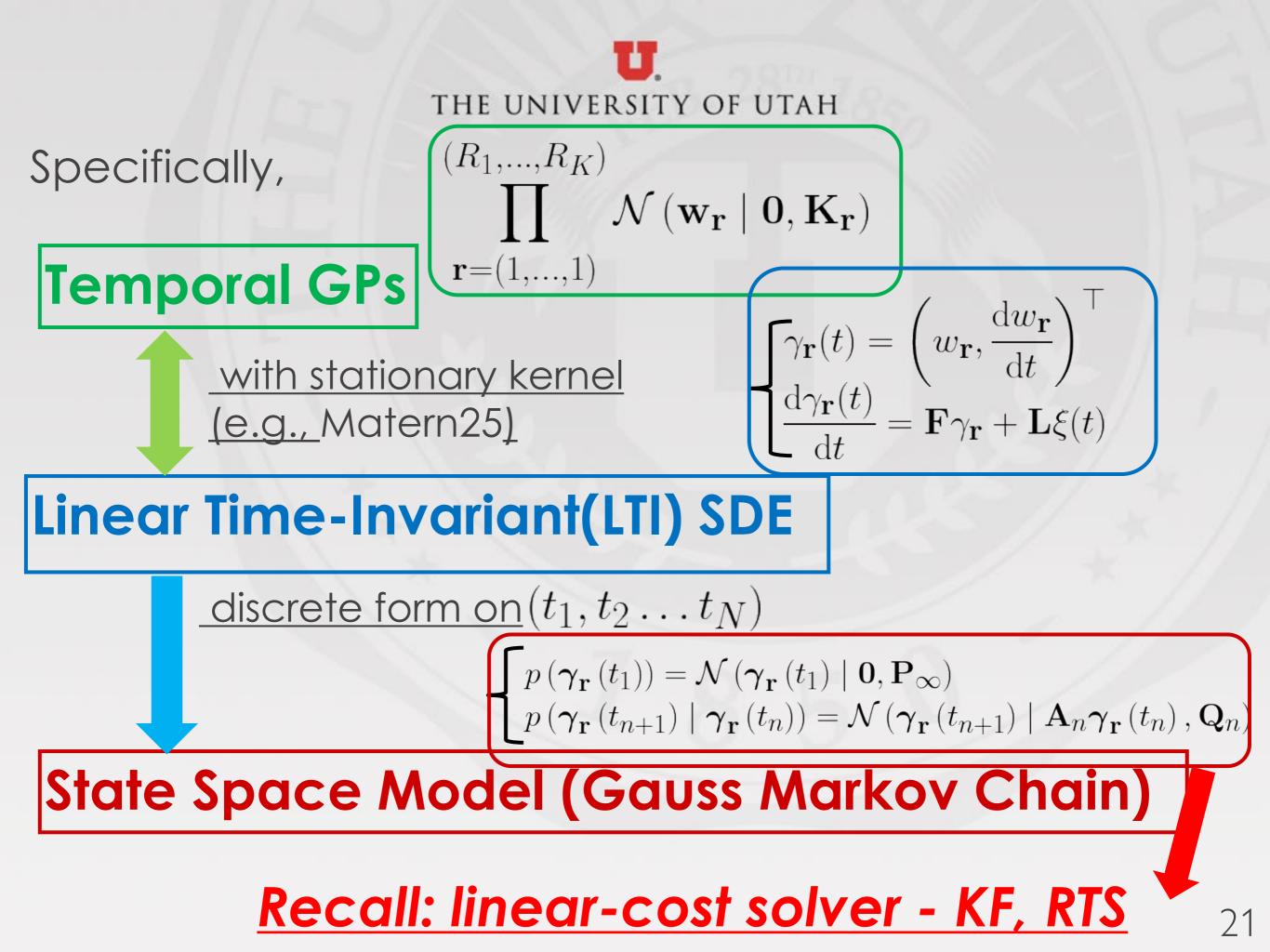


*: it holds with linear emission/observed likelihood, if with non-linear, we could apply non-linear filter and smoothing 19



Illustration of computation cost:







Reformulate Tucker core with State Space Priors

$$p(\bar{\gamma}_1) \prod_{n=1}^{N-1} p(\bar{\gamma}_{n+1} \mid \bar{\gamma}_n)$$

We post Gaussian-Gamma Approx. to fit each data-llk $\mathcal{N}\left(y_n \mid (\mathbf{H}\bar{\gamma}_n)^\top \left(\mathbf{u}_{i_{n_1}}^1 \otimes \ldots \otimes \mathbf{u}_{i_nK}^K\right), \tau^{-1}\right) \approx$ $Z_n \prod_{k=1}^K \mathcal{N}\left(\mathbf{u}_{i_{n_k}}^k \mid \mathbf{m}_{i_{n_k}}^{k,n}, \mathbf{V}_{i_{n_k}}^{k,n}\right) \cdot \operatorname{Gam}\left(\tau \mid b_n, c_n\right) \text{Approx. Msg of Factors & noise}$ $\times \mathcal{N}\left(\mathbf{H}\bar{\gamma}_n \mid \boldsymbol{\beta}_n, \mathbf{S}_n\right) \quad \text{Approx. Msg of SDE states} \text{/Tucker core}$

Substitute these into joint prob.



The proposed approx. posterior is:

$$q\left(\mathcal{U},\left\{\bar{\gamma}_{n}\right\},\tau\right) \propto \prod_{k=1}^{K} \prod_{j=1}^{d_{k}} \mathcal{N}\left(\mathbf{u}_{j}^{k} \mid \mathbf{0},\mathbf{I}\right) \operatorname{Gam}\left(\tau \mid b_{0},c_{0}\right)$$
Standard moment match? Infeasible!

$$\prod_{n=1}^{N} \prod_{k=1}^{K} \mathcal{N}\left(\mathbf{u}_{i_{n_{k}}}^{k} \mid \mathbf{m}_{i_{n_{k}}}^{k,n}, \mathbf{V}_{i_{n_{k}}}^{k,n}\right) \operatorname{Gam}\left(\tau \mid b_{n},c_{n}\right)$$

$$p\left(\bar{\gamma}_{1}\right) \mathcal{N}\left(\mathbf{H}\bar{\gamma}_{1} \mid \boldsymbol{\beta}_{1}, \mathbf{S}_{1}\right) \prod_{n=1}^{N-1} p\left(\bar{\gamma}_{n+1} \mid \bar{\gamma}_{n}\right) \mathcal{N}\left(\mathbf{H}\bar{\gamma}_{n} \mid \boldsymbol{\beta}_{n}, \mathbf{S}_{n}\right)$$
SDE states: Solve by KF and RTS Apply conditional moment matching and delta method!



Conditional Moment Match

$$\mathbb{E}_{\widetilde{p}}[\phi(\boldsymbol{\eta}_n)] = \mathbb{E}_{\widetilde{p}(\Theta_{\backslash \eta_n})} \left[\mathbb{E}_{\widetilde{p}(\boldsymbol{\eta}_n | \Theta_{\backslash \eta_n})} \left[\phi(\boldsymbol{\eta}) \mid \Theta_{\backslash \boldsymbol{\eta}_n} \right] \right]$$

• Delta method:

$$\mathbb{E}_{q\left(\Theta_{\backslash \eta_{n}}\right)}\left[\boldsymbol{\rho}_{n}\right] \approx \rho_{n}\left(\mathbb{E}_{q}\left[\boldsymbol{\Theta}_{\backslash \boldsymbol{\eta}_{n}}\right]\right)$$

Enable **tractable moment matching** to update approx. probability terms under Expectation Propagation(EP) framework



Algorithm 1 BCTT

Input: $\mathcal{D} = \{(\mathbf{i}_1, t_1, y_1), \dots, (\mathbf{i}_N, t_N, y_N)\}, \text{ kernel hyper-parameters } l, \sigma^2$

Initialize approximation terms in (10) for each likelihood. **repeat**

Run KF and RTS smoothing to compute each $q(\overline{\gamma}_n)$ for n = 1 to N in parallel do

Simultaneously update $\mathcal{N}(\mathbf{H}\overline{\gamma}_{n}|\boldsymbol{\beta}_{n}, \mathbf{S}_{n})$, $Gam(\tau|b_{n}, c_{n})$ and $\left\{\mathcal{N}\left(\mathbf{u}_{i_{n_{k}}}^{k}|\mathbf{m}_{i_{n_{k}}}^{k,n}, \mathbf{V}_{i_{n_{k}}}^{k,n}\right)\right\}_{k}$ in (10) with conditional moment matching and multi-variate delta method.

end for

until Convergence

Return: $\{q(\mathcal{W}(t_n))\}_{n=1}^N, \{q(\mathbf{u}_j^k)\}_{1 \le k \le K, 1 \le j \le d_k}, q(\tau)$

Time cost: $\mathcal{O}(N\bar{R})$ **Space cost:** $\mathcal{O}\left(N\left(\bar{R}^2 + \sum_{k=1}^K R_k^2\right)\right)$



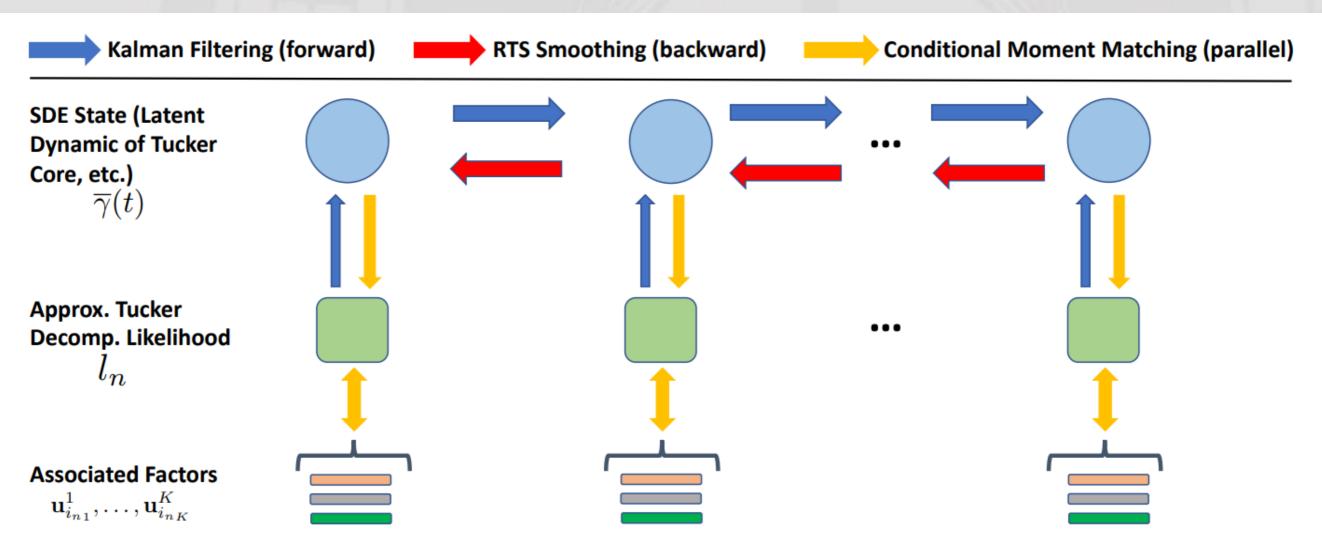
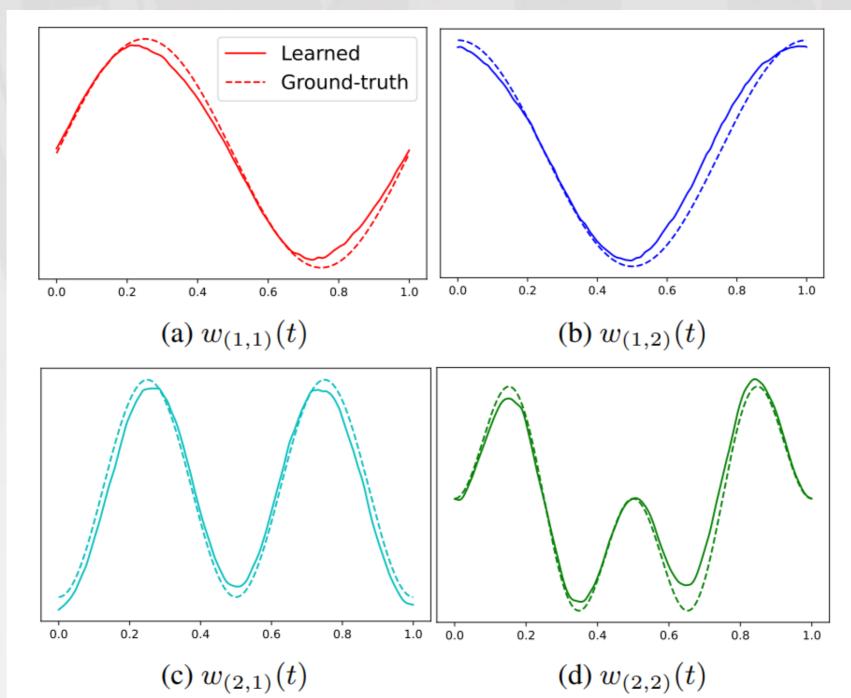


Figure 1. Graphical illustration of the message-passing inference algorithm.



Can BCTT capture the temporal patterns in tensor?

- Exp on simulation data
- Plot the dynamics of Tucker core



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Can BCTT capture the temporal patterns in tensor?

- Exp on real-world data(DBLP dataset)
- Scatter low-rank structures of Tucker core

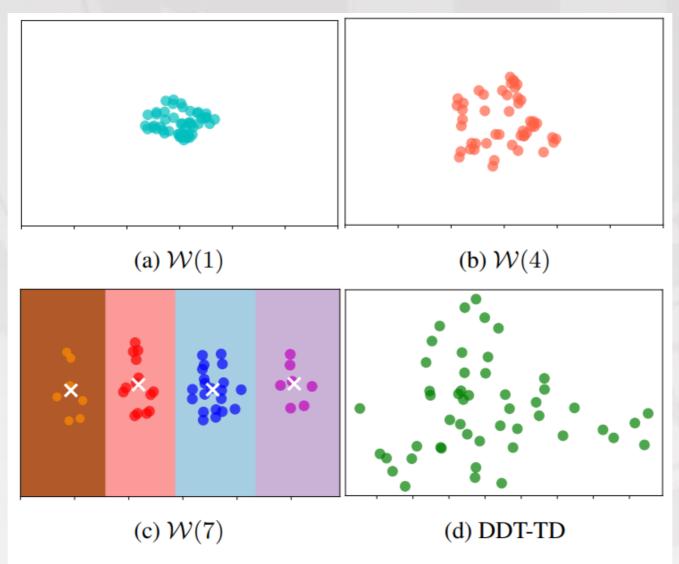


Figure 4. The structures of learned tensor-core at different time points by BCTT (a-c) and the static tensor-score learned by dynamic discrete-time Tucker decomposition (DDT-TD).

U. The University of Utah

Prediction with BCTT

• Prediction performance of BCTT on 3 real-world data

RMSE	MovieLens	AdsClicks	DBLP	RMSE	MovieLens	AdsClicks	DBLP
CT-CP	1.113 ± 0.004	1.337 ± 0.013	0.240 ± 0.007	CT-CP	1.165 ± 0.008	1.324 ± 0.013	0.263 ± 0.0
CT-GP	0.949 ± 0.008	1.422 ± 0.008	0.227 ± 0.009	CT-GP	0.965 ± 0.019	1.410 ± 0.015	0.227 ± 0.0
DT-GP	0.963 ± 0.008	1.436 ± 0.015	0.227 ± 0.007	DT-GP	0.949 ± 0.007	1.425 ± 0.015	0.225 ± 0.00
DDT-GP	0.957 ± 0.008	1.437 ± 0.010	0.225 ± 0.006	DDT-GP	0.948 ± 0.005	1.421 ± 0.012	0.220 ± 0.00
DDT-CP	1.022 ± 0.003	1.420 ± 0.020	0.245 ± 0.004	DDT-CP	1.141 ± 0.007	1.623 ± 0.013	0.282 ± 0.02
DDT-TD	1.059 ± 0.006	1.401 ± 0.022	0.232 ± 0.09	DDT-TD	0.944 ± 0.003	1.453 ± 0.035	$0.312\pm0.0^{\prime}$
BCTT	0.922 ± 0.002	1.322 ± 0.012	0.214 ± 0.009	BCTT	0.895 ± 0.007	1.304 ± 0.018	0.202 ± 0.0
MAE				MAE			
CT-CP	0.788 ± 0.004	0.787 ± 0.006	0.105 ± 0.001	CT-CP	0.835 ± 0.006	0.792 ± 0.007	0.128 ± 0.00
CT-GP	0.714 ± 0.004	0.891 ± 0.011	0.092 ± 0.004	CT-GP	0.717 ± 0.012	0.883 ± 0.016	0.092 ± 0.0
DT-GP	0.722 ± 0.008	0.893 ± 0.008	0.084 ± 0.003	DT-GP	0.714 ± 0.005	0.886 ± 0.012	0.084 ± 0.00
DDT-GP	0.720 ± 0.003	0.894 ± 0.009	0.083 ± 0.001	DDT-GP	0.707 ± 0.004	0.882 ± 0.015	0.082 ± 0.00
DDT-CP	0.755 ± 0.002	0.901 ± 0.011	0.114 ± 0.002	DDT-CP	0.843 ± 0.003	1.082 ± 0.013	0.141 ± 0.00
DDT-TD	0.742 ± 0.006	0.866 ± 0.012	0.101 ± 0.001	DDT-TD	0.712 ± 0.002	0.903 ± 0.024	0.221 ± 0.04
BCTT	0.698 ± 0.002	0.777 ± 0.016	0.084 ± 0.001	BCTT	0.679 ± 0.001	0.785 ± 0.010	0.080 ± 0.0

(a) R = 3

(b) R = 7



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Shikai Fang, Robert. M. Kirby, and Shandian Zhe, "Bayesian Streaming Sparse Tucker Decomposition", The 37th Conference on Uncertainty in Artificial Intelligence (UAI), 2021



• Sparsity in tensor data requires Sparsity in model

Tensor-Datasets	Size	#Observed entries	Observed Ratio
Gowalla	18737*1000*32510	821,931	0.0001%
SG	2321*5596*1600	105,764	0.0005%
ACC	3000*150*30000	1,220,000	0.1%
Movielens1M	6000*3700	1,000,000	4%

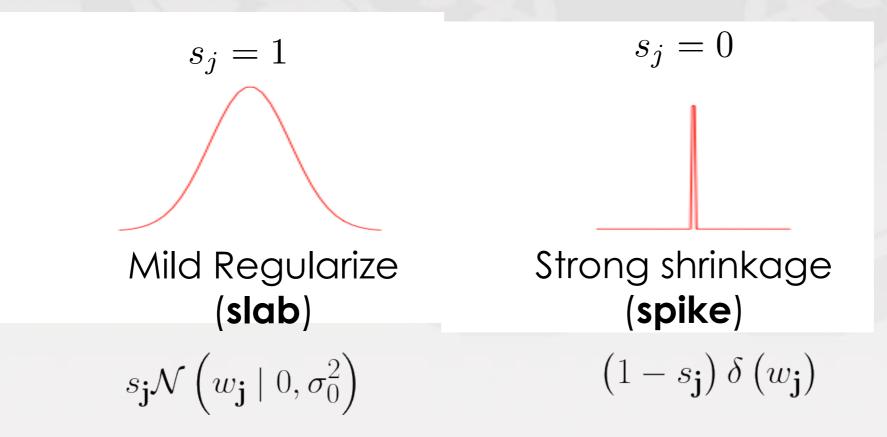
- otherwise, overfitting risk, especially for complex model like NN
- How non-Bayesian people get sparsity?
 --L1 regular terms
 --overall sparse, not accurate enough



How Bayesian people get sparsity?

Spike and Slab Priors

Introduce binary selection indicators s_1, s_2, \ldots, s_d on each parameter ! -- Element-wise sparse control!

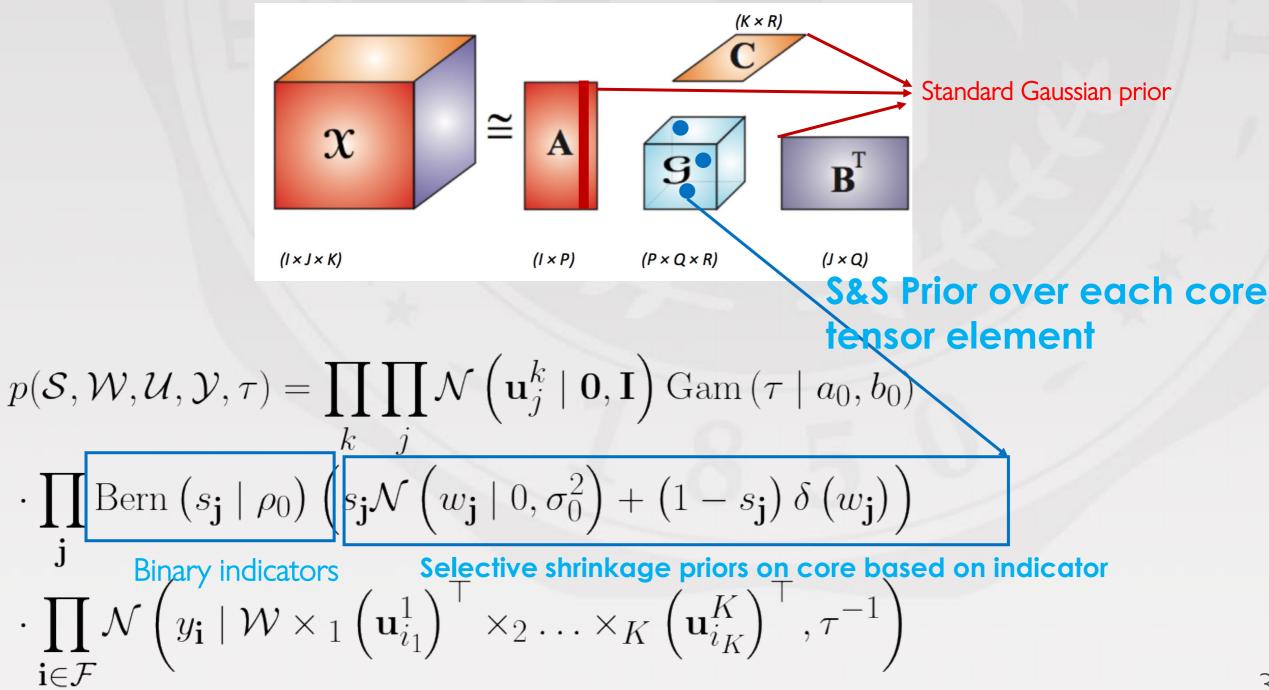




Where to put such sparsity?

 $\mathbf{i} \in \mathcal{F}$

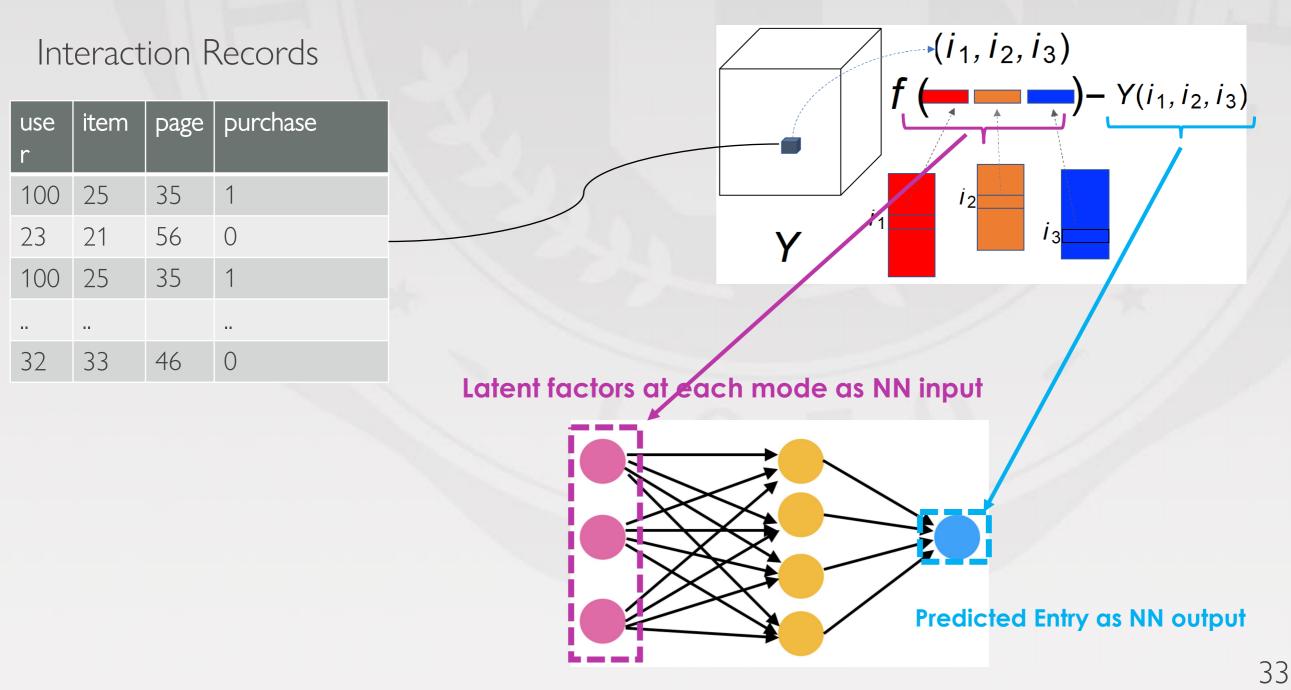
On Tucker Core-build a sparse core (BASS[4])



[5] Fang, Shikai, et al. "Bayesian Streaming Sparse Tucker decomposition." Conference on Uncertainty in Artificial Intelligence. UAI, 2021



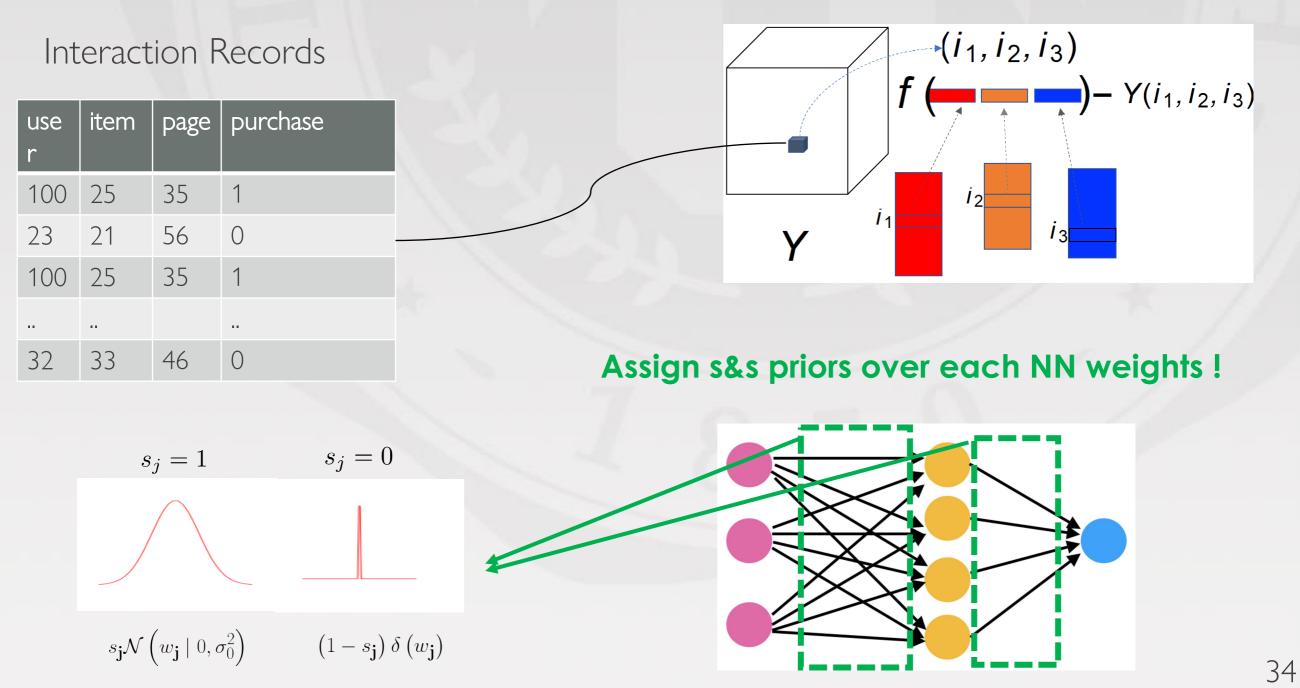
Where to put such sparsity? On NN weights – build a sparse BNN (SBDT[4])



[4] Fang, Shikai, et al. "Streaming Probabilistic Deep Tensor Factorization." The Thirty-eighth International Conference on Machine Learning (ICML), 2021



Where to put such sparsity? On NN weights – build a sparse BNN (SBDT[4])



[4] Fang, Shikai, et al. "Streaming Probabilistic Deep Tensor Factorization." The Thirty-eighth International Conference on Machine Learning (ICML), 2021



How the final sparsity exactly look like?

 Approx. of S&S Priors in exponential family: Gaussian + Bernoulli

 $p\left(w_{mjt} \mid s_{mjt}\right) \propto A\left(w_{mjt}, s_{mjt}\right)$ $= \operatorname{Bern}\left(s_{mjt} \mid c\left(\rho_{mjt}\right)\right) \mathcal{N}\left(w_{mjt} \mid \mu_{mjt}^{0}, v_{mjt}^{0}\right)$

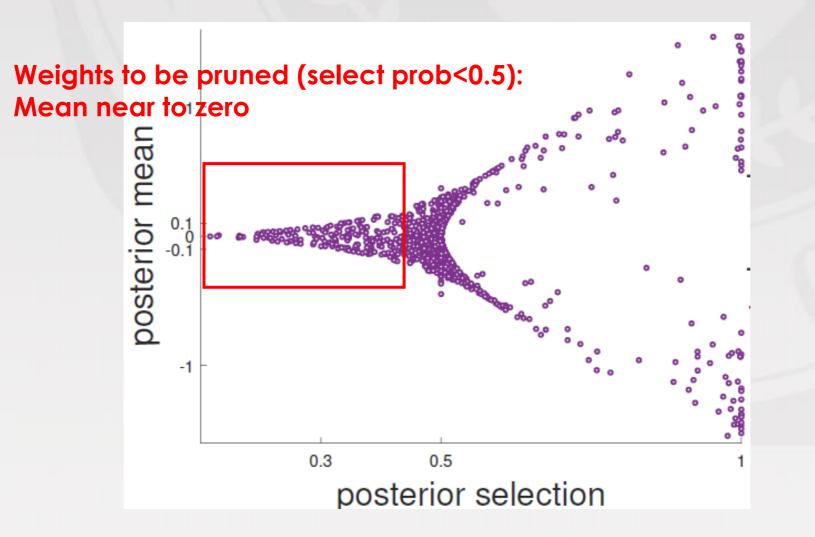
Select posterior prob of each weight <0.5: unselected <=> sparse



• How sparse can model get? – Light model

For SBDT work (Sparse BNN as factorization model)

- Plot of sparse-BNN weights after training
- Each weight has its posterior mean, var and selection prob.



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- How sparse can model get? Interpretability
 For BASS work (Tucker with Sparse core as factorization model)
- Plot of projected Tucker core elements with sparsity
- Significant structure of interactions

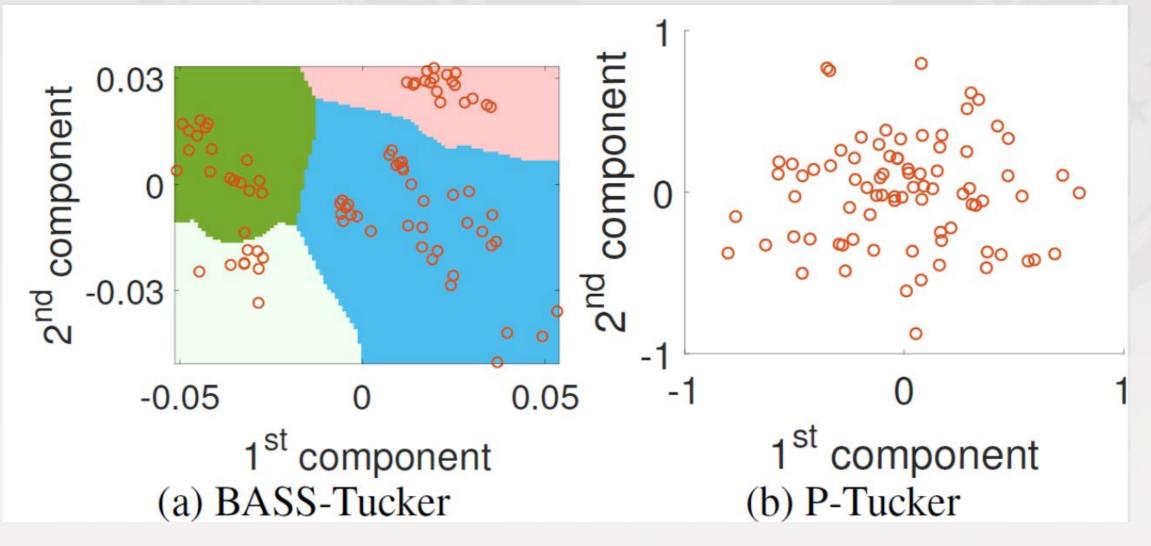


Image: Fang, Shikai, et al. "Bayesian Streaming Sparse Tucker decomposition." Conference on Uncertainty in Artificial Intelligence. UAI, 2021.

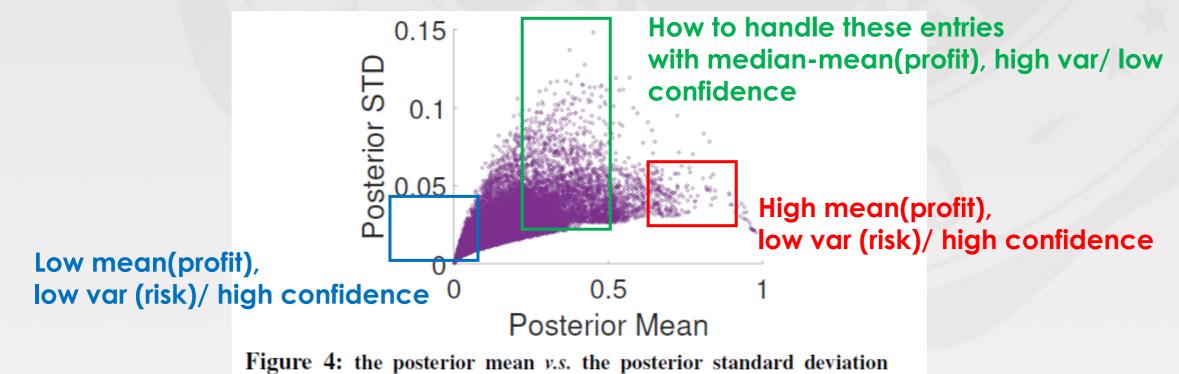
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How to make use of quantized uncertainty?

An example in ad-recommend system

- plots of model predictions on CTR(click-through-rate) tensor dataset
- exploration and exploitation, optimization policy for down steaming tasks



(STD) of the click probability prediction.

Image from Conor Tillinghast, Shikai Fang, Kai Zheng, and Shandian Zhe, "Probabilistic Neural-Kernel Tensor Decomposition", IEEE International Conference on Data 37 Mining (ICDM), 2020.



Open questions for Cooperation

- Domain knowledge embedded in prior
- Make good use of the uncertainty measure
- Challenges and inspiration from real world

Domain model(PDE/SDE) + Al4Science + new algos...



Thanks for attention Q&A Time

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Webpage: https://www.cs.utah.edu/~shikai/

Focus: Bayesian machine learning, tensor learning

知乎:方轩固