

Rethinking Sparsity-Aware Bayesian Learning for Signal Processing and Machine Learning

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Overview

- 1 Motivation of Sparsity-Aware Learning
- 2 Sparsity-Aware Learning: from Frequentist to Bayesian
- 3 Sparsity-Aware Gaussian Process Models
- 4 Sparsity-Aware Bayesian Neural Network Models
- 5 Sparsity-Aware Tensor Decomposition Models
- 6 Applications of Modern Sparsity-Aware Models
- 7 Conclusion and Future Directions

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Background

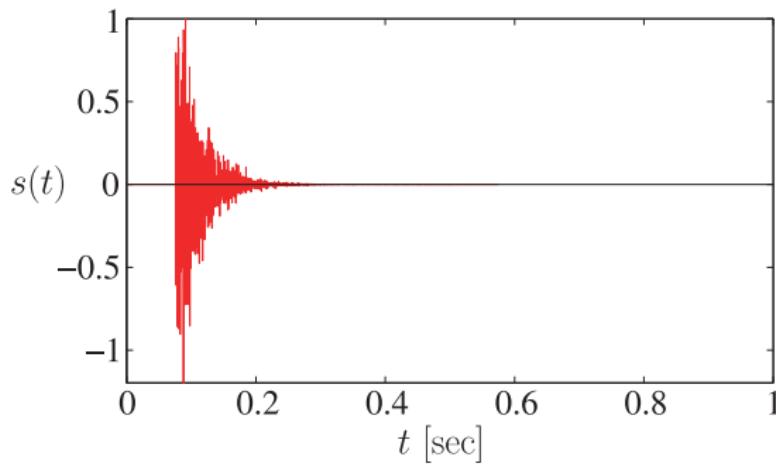
- Sparsity-aware learning has offered novel theoretical tools and solutions to challenging practical problems in various sectors.
- Applications include biomedicine, astronomy, signal processing, wireless communications, and data science.
- Sparsity-aware learning can be achieved from either a Frequentist path or a Bayesian path.

Sparsity-aware learning is capable of

- improving the overall parameter estimation performance (in terms of bias and variance);
- guarding against over-fitting, particularly when data samples are scarce;
- coping with ill-conditions, such as rank-deficient covariance matrices,etc;
- providing a solution to underdetermined linear system of equations;
- generating parsimonious models with sparse and interpretable signal representation.

Classic Examples: Echo Path Representation

- Sparsity is an attribute that is met in a plethora of natural signals, because **nature tends to be parsimonious**.
- Echo path vector comprising the values of impulse response samples **is sparse**.

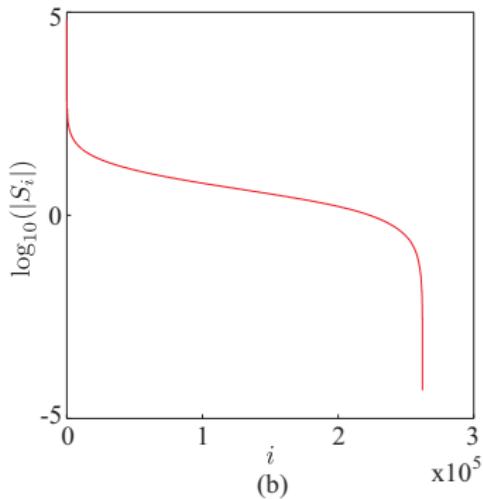


Impulse response function of an echo path in a telephone network. **Short duration and no prior knowledge about its appearance in time.**

Classic Examples: Image Compression



(a)



(b)

(a) A 512×512 image; and (b) the magnitude of its discrete cosine transform (DCT) components in descending order.

- **Heart of compression:** More than 95% of the total energy contributed by only 5% of the largest components.

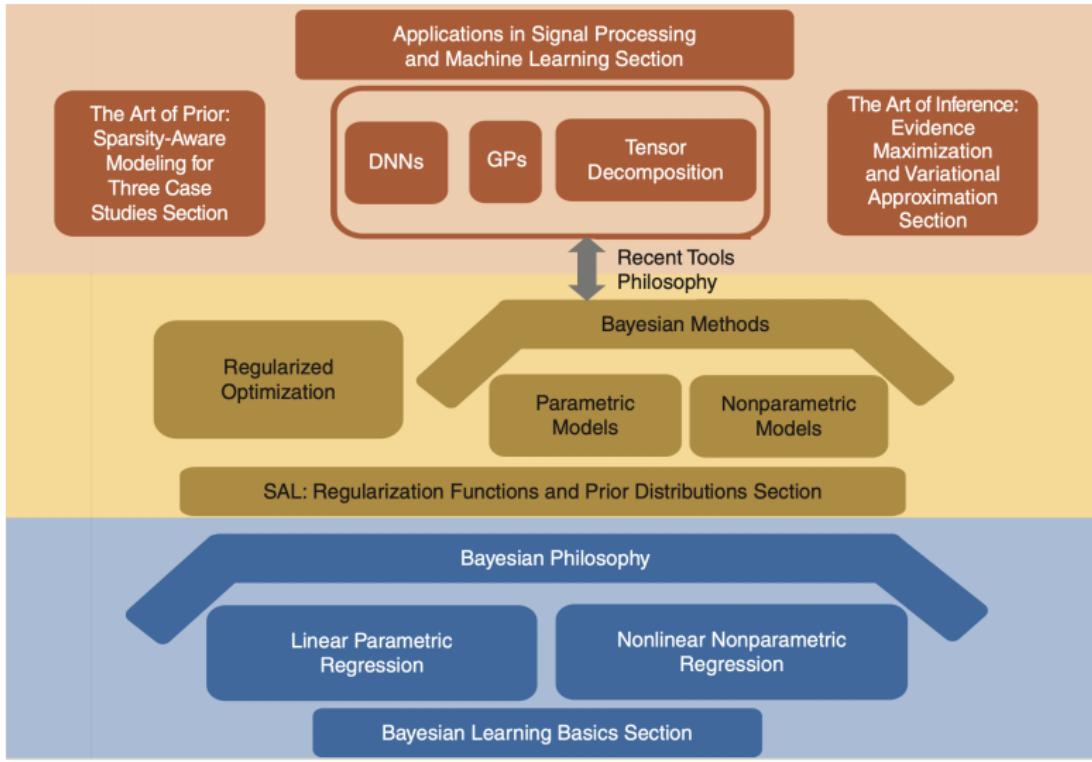
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- This tutorial will focus on sparsity-aware learning via Bayesian path.
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- This tutorial will show sparsity-promoting priors and inference strategies for modern Gaussian process, Bayesian neural network, and tensor decomposition models.
- This tutorial was prepared mainly based on:
 - ① L. Cheng, F. Yin, S. Theodoridis, S. Chatzis and T. -H. Chang, "Rethinking Bayesian Learning for Data Analysis: The art of prior and inference in sparsity-aware modeling," in IEEE Signal Processing Magazine, vol. 39, no. 6, pp. 18-52, Nov. 2022.
 - ② Sergios Theodoridis, "Machine Learning: A Bayesian and Optimization Perspective", Academic Press, 2nd Edition, 2020.

Organization



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Section Goals

This section aims to

- provide some **basics about Bayesian learning philosophy**;
- introduce important **notations and quantities** of Bayesian learning;
- introduce Bayesian **parametric** and **nonparametric models**.

Brief Review of Frequentist Path

In the past, more dominantly, sparsity-aware learning was conducted via regularized optimization of the general form:

$$\hat{\boldsymbol{\theta}} = \arg \min_{\boldsymbol{\theta}} \ell(\mathcal{D}; \boldsymbol{\theta}) + \lambda \cdot r(\boldsymbol{\theta}),$$

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$$\hat{\theta} = \arg \min_{\theta} \ell(\mathcal{D}; \theta) + \lambda \cdot r(\theta),$$

where

- θ represents the desired model parameters;
- $\ell(\mathcal{D}; \theta)$ is a cost function w.r.t. a finite dataset, $\mathcal{D} \triangleq \{\mathbf{y}, \mathbf{X}\}$, to measure the data fitting performance;
- $r(\theta)$ is a regularization function w.r.t. the model parameters, θ , to steer the sparsity structure embedding;
- λ is a regularization parameter to balance data fitting and sparsity structure embedding.

RIDGE Regression vs. LASSO Regression

- RIDGE regression adopts least-squares loss and ℓ_2 norm as regularization,

$$\hat{\boldsymbol{\theta}}_R = \arg \min_{\boldsymbol{\theta}} \left((\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) + \lambda \|\boldsymbol{\theta}\|_2 \right).$$

- RIDGE regression admits a closed-form solution:

$$\hat{\boldsymbol{\theta}}_R = \left(\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I} \right)^{-1} \mathbf{X}^T \mathbf{y}.$$

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- The solution has no sparsity structure.

- LASSO regression adopts least-squares loss but ℓ_1 norm as regularization,

$$\hat{\boldsymbol{\theta}}_L = \arg \min_{\boldsymbol{\theta}} \left((\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) + \lambda \|\boldsymbol{\theta}\|_1 \right).$$

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- LASSO regression can be equivalently written as

$$\begin{aligned} \hat{\boldsymbol{\theta}}_L = & \arg \min_{\boldsymbol{\theta}} (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) \\ \text{s.t. } & \|\boldsymbol{\theta}\|_1 \leq \rho \end{aligned}$$

or (also known as basis pursuit denoising)

$$\begin{aligned} \hat{\boldsymbol{\theta}}_L = & \arg \min_{\boldsymbol{\theta}} \|\boldsymbol{\theta}\|_1 \\ \text{s.t. } & (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) \leq \epsilon \end{aligned}.$$

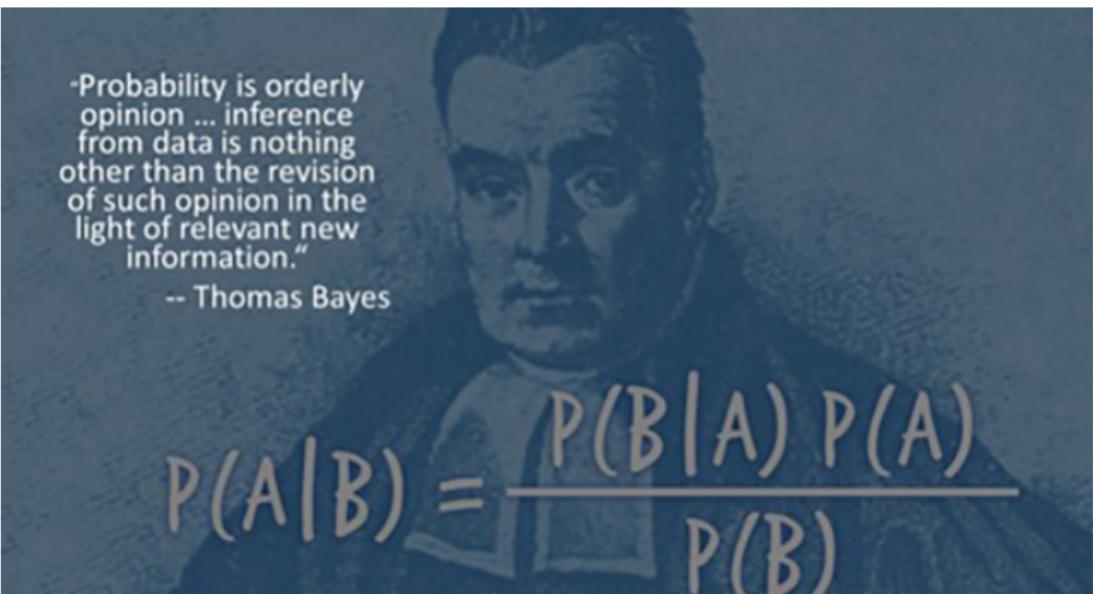
- The solution requires iterative algorithms but shows sparsity structure.

References for Frequentist Path

- Chapter 9 and 10 of *Machine Learning: A Bayesian and Optimization Perspective* by Sergios Theodoridis.
- Chapter 13 of *Machine Learning: A Probabilistic Perspective* by Kevin P. Murphy.
- Various Tutorials given at NeurIPS, ICLR, AAAI,etc, in the past five years.

The Heart of Bayesian Learning

In this tutorial, we will rethink sparsity-aware learning via the Bayesian path paved by the elegant and generic Bayes' Theorem.

A portrait of Thomas Bayes, an English statistician and Presbyterian minister, looking slightly to the right. He has dark hair and is wearing a dark coat over a white collar.

-Probability is orderly opinion ... inference from data is nothing other than the revision of such opinion in the light of relevant new information."

-- Thomas Bayes

$$P(A|B) = \frac{P(B|A) P(A)}{P(B)}$$

Notations

- Let \mathcal{D} be the observed (training) dataset.
- Let \mathcal{M} be the underlying model for having generated the data.
- Let $\theta \in \mathbb{R}^{L \times 1}$ be the unknown model parameters, treated as **random variables**.
- Let $\theta \sim p_{\mathcal{M}}(\theta; \eta_p)$ be the **prior distribution** of θ .
- Let η_p be a set of deterministic yet unknown **hyperparameters** to specify the prior.
- Let $p_{\mathcal{M}}(\mathcal{D}|\theta)$ be the **likelihood** to describe the observed data given the values of the parameters.

Bayes' Theorem and Important Quantities

$$p_{\mathcal{M}}(\boldsymbol{\theta}|\mathcal{D}; \boldsymbol{\eta}) = \frac{p_{\mathcal{M}}(\mathcal{D}|\boldsymbol{\theta})p_{\mathcal{M}}(\boldsymbol{\theta}; \boldsymbol{\eta}_p)}{p_{\mathcal{M}}(\mathcal{D}; \boldsymbol{\eta})},$$

where

- **Prior:** $p_{\mathcal{M}}(\boldsymbol{\theta}; \boldsymbol{\eta}_p)$
- **Likelihood:** $p_{\mathcal{M}}(\mathcal{D}|\boldsymbol{\theta})$
- **Posterior:** $p_{\mathcal{M}}(\boldsymbol{\theta}|\mathcal{D}; \boldsymbol{\eta})$
- **Evidence/Marginal Likelihood:** $p_{\mathcal{M}}(\mathcal{D}; \boldsymbol{\eta})$

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-
- **Evidence** is computed as the **marginalization of the likelihood**:

$$p_{\mathcal{M}}(\mathcal{D}; \boldsymbol{\eta}) = \int p_{\mathcal{M}}(\mathcal{D}|\boldsymbol{\theta})p_{\mathcal{M}}(\boldsymbol{\theta}; \boldsymbol{\eta}_p)d\boldsymbol{\theta}.$$

- **Classic ML estimator** can be obtained via:

$$\hat{\boldsymbol{\eta}}_{ML} = \arg \max_{\boldsymbol{\eta}} \log p_{\mathcal{M}}(\mathcal{D}; \boldsymbol{\eta})$$

Evidence vs. ELBO

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$$\log p_{\mathcal{M}}(\mathcal{D}; \boldsymbol{\eta}) \geq \mathcal{L}(q(\boldsymbol{\theta}); \boldsymbol{\eta}) \triangleq \int q(\boldsymbol{\theta}) \log \frac{p_{\mathcal{M}}(\mathcal{D}, \boldsymbol{\theta}; \boldsymbol{\eta})}{q(\boldsymbol{\theta})} d\boldsymbol{\theta}.$$

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- Tightness of ELBO is determined by the closeness between the variational distribution $q(\boldsymbol{\theta})$ and the posterior $p_{\mathcal{M}}(\boldsymbol{\theta}|\mathcal{D}; \boldsymbol{\eta})$.
- Solving ELBO maximization problem for different learning models:

$$\max_{q(\boldsymbol{\theta}), \boldsymbol{\eta}} \mathcal{L}(q(\boldsymbol{\theta}); \boldsymbol{\eta}).$$

Parametric Model vs. Nonparametric Model

- Parametric Model:

- ① adopts a finite set of parameters θ ,
- ② outputs point estimate solely relying on the model parameters trained based on the observed data, \mathcal{D} ,
- ③ Bayesian linear regression model is a represented one.

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- **Nonparametric Model:**

- ① adopts an infinite dimensional θ , often regarded as a random function,
- ② keeps updating θ as data \mathcal{D} expands with finer granularity,
- ③ Gaussian process model is a represented one.

Parametric Model: Bayesian Linear Regression

We start with the ordinary linear regression model:

$$y_n = f(\mathbf{x}_n; \boldsymbol{\theta}) + v_n, \quad n = 1, 2, \dots, N.$$

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where the regression function is

$$f(\mathbf{x}; \boldsymbol{\theta}) = \boldsymbol{\theta}^T \mathbf{x},$$

and

- $\mathbf{x} = [x_1, x_2, \dots, x_L]^T$ is the input/feature vector of size L ,
- $\boldsymbol{\theta}$ is the vector of model parameters following certain distribution,
- $v_n, n = 1, 2, \dots, N$ are independent noise terms.

Classically, by assuming:

- Gaussian likelihood, owing to $\{v_n\} \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(v_n; 0, \beta^{-1})$, where β represents the noise precision, and

$$p_{\mathcal{M}}(\mathcal{D}|\theta) = \prod_{n=1}^N \mathcal{N}(y_n; \theta^T \mathbf{x}_n, \beta^{-1}).$$

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$$p_{\mathcal{M}}(\mathcal{D}|\theta) = \prod_{n=1}^N \mathcal{N}(y_n; \theta^T \mathbf{x}_n, \beta^{-1}).$$

- Gaussian prior on the unknown parameters,

$$p_{\mathcal{M}}(\theta; \eta_p) = \prod_{l=1}^L \mathcal{N}(\theta_l; 0, \alpha_l^{-1}),$$

where α_l is the precision for θ_l , and $\eta_p \triangleq [\alpha_1, \alpha_2, \dots, \alpha_L]^T$.

We can derive then two important quantities:

- Gaussian evidence obtained through marginalization:

$$\begin{aligned} p_{\mathcal{M}}(\mathcal{D}; \boldsymbol{\eta}) &= \int p_{\mathcal{M}}(\mathcal{D}|\boldsymbol{\theta}) p_{\mathcal{M}}(\boldsymbol{\theta}; \boldsymbol{\eta}_p) d\boldsymbol{\theta} \\ &= \mathcal{N}(\mathbf{y}; \mathbf{0}, \beta^{-1} \mathbf{I} + \mathbf{X} \mathbf{A}^{-1} \mathbf{X}^T), \end{aligned}$$

where $\mathbf{A} \triangleq \text{diag}\{\alpha_1, \alpha_2, \dots, \alpha_L\}$ and $\boldsymbol{\eta} = [\boldsymbol{\eta}_p^T, \beta]^T$.

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- Gaussian posterior eventually derived from Bayes' theorem:

$$p_{\mathcal{M}}(\boldsymbol{\theta}|\mathcal{D}; \boldsymbol{\eta}) = \mathcal{N}(\boldsymbol{\theta}; \boldsymbol{\mu}, \boldsymbol{\Sigma}),$$

where

$$\begin{aligned} \boldsymbol{\mu} &= \beta \boldsymbol{\Sigma} \mathbf{X}^T \mathbf{y}, \\ \boldsymbol{\Sigma} &= (\mathbf{A} + \beta \mathbf{X}^T \mathbf{X})^{-1}. \end{aligned}$$

Often, point prediction is obtained by $y_* = \boldsymbol{\mu}^T \mathbf{x}_*$.

Nonparametric Model: Gaussian Process Regression

A representative example of Bayesian nonparametric model is the [Gaussian process model for machine learning](#) with the definitions:

Definition 1: Gaussian process [Rasmussen, 2006]⁰

A Gaussian process is a collection of random variables, any finite number of which have a joint Gaussian distribution.

⁰C.Rasmussen and C.Williams, Gaussian Process for Machine Learning, MIT Press,2006. A set of small, light-blue navigation icons typically used in Beamer presentations for navigating between slides and sections.

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Definition 2: Gaussian process [Theodoridis, 2020]

A random process, $f(\mathbf{x})$, is called a Gaussian process if and only if for any finite number of points, $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N$, the associated joint probability density function (pdf), $p(f(\mathbf{x}_1), f(\mathbf{x}_2), \dots, f(\mathbf{x}_N))$ is Gaussian.

⁰C.Rasmussen and C.Williams, Gaussian Process for Machine Learning, MIT Press,2006.

- A real GP, $f(\mathbf{x})$, is completely specified by its **mean function** $m(\mathbf{x})$ and its **covariance function/kernel function** $k(\mathbf{x}, \mathbf{x}')$ as

$$m(\mathbf{x}) \triangleq \mathbb{E}[f(\mathbf{x})],$$

$$k(\mathbf{x}, \mathbf{x}') \triangleq \mathbb{E}[(f(\mathbf{x}) - m(\mathbf{x})) (f(\mathbf{x}') - m(\mathbf{x}'))].$$

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$$k(\mathbf{x}, \mathbf{x}') \triangleq \mathbb{E}[(f(\mathbf{x}) - m(\mathbf{x})) (f(\mathbf{x}') - m(\mathbf{x}'))].$$

- We denote a GP as

$$f(\mathbf{x}) \sim \mathcal{GP}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}'; \boldsymbol{\eta}_p)).$$

- Model representation power is determined to large extent by the kernel function.

Kernel Functions

- Every specification of a kernel function determines to a family of functions.
- Some elementary kernel functions are:

- ① Linear kernel (with $\eta_p = \sigma_0$)

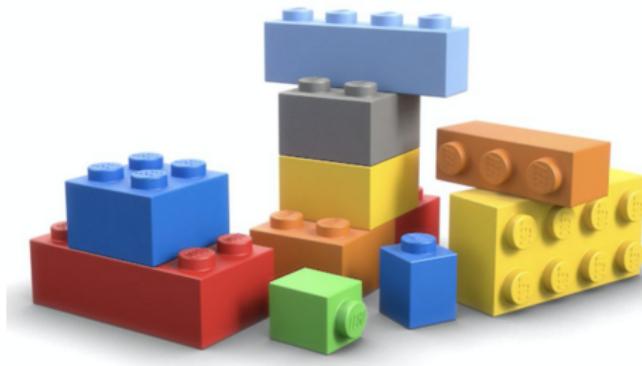
$$k(\mathbf{x}, \mathbf{x}'; \eta_p) = \sigma_0 + \mathbf{x}^T \mathbf{x}'$$

- ② Squared Exponential (SE)/Gaussian kernel (with $\eta_p = [\sigma_s^2, \ell_s]^T$)

$$k(\mathbf{x}, \mathbf{x}'; \eta_p) = \sigma_s^2 \exp\left(-\frac{\|\mathbf{x} - \mathbf{x}'\|^2}{2\ell_s^2}\right)$$

- ③ Matern kernels, rational quadratic kernels, periodic kernels, local periodic kernels, etc.

Kernel Selection and Design



Many elementary kernel functions available

We focus on a class of interpretable and sparsity-promoting kernel functions to form a GP prior.

Gaussian Process for Regression

We consider the following **GP regression** model

$$y = f(\mathbf{x}) + \varepsilon,$$

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We consider the following GP regression model

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where

- y is a continuous-valued scalar output;
- the underlying regression function is represented by a zero-mean Gaussian process $f(\mathbf{x})$ specified by $k(\mathbf{x}, \mathbf{x}'; \boldsymbol{\eta}_p)$;
- the noise terms are Gaussian i.i.d. with zero-mean and unknown variance β^{-1} ;
- The set of all unknown parameters, $\boldsymbol{\eta} = [\boldsymbol{\eta}_p, \beta]^T$.

- Given a finite number of training input points: $X = [\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n]$, $\mathbf{y} = [y_1, y_2, \dots, y_n]^T$.
- The selected Gaussian process prior boils down to a multivariate Gaussian distribution, with

$$\mathbf{f} := [f(\mathbf{x}_1), f(\mathbf{x}_2), \dots, f(\mathbf{x}_n)]^T \sim \mathcal{N}(\mathbf{0}, K(X, X)).$$

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- The likelihood function, given \mathbf{f} , is also Gaussian of the form:

$$p(\mathbf{y}|\mathbf{f}; \boldsymbol{\eta}) = \mathcal{N}(\mathbf{y}; \mathbf{f}, \beta^{-1} \mathbf{I}_n).$$

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Recall Fundamental Tasks

- Kernel selection/design
- Kernel hyperparameter optimization
- Posterior prediction of novel data points

Task: Kernel Hyperparameter Optimization

- Conventionally, hyperparameters η , are derived from **maximizing the evidence**.
- Due to Gaussian process prior and Gaussian likelihood function, the **evidence in closed-form** can be derived as:

$$p(\mathbf{y}; \boldsymbol{\eta}) = \mathcal{N}(\mathbf{y}; \mathbf{0}, \mathbf{K}(X, X; \boldsymbol{\eta}_p) + \beta^{-1} \mathbf{I}).$$

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- Such optimization problem is typically **smooth but non-convex** for general regression and classification problems.
- Inaccurate prediction will incur when a **bad local optimum** is found by gradient descent type of methods.

Task: Posterior Prediction

- **Goal:** To predict $\mathbf{y}_* = [y_{*,1}, y_{*,2}, \dots, y_{*,n_*}]^T$ given novel (test) inputs $X_* = [\mathbf{x}_{*,1}, \mathbf{x}_{*,2}, \dots, \mathbf{x}_{*,n_*}]$ from its **posterior distribution** $p(\mathbf{y}_* | \mathcal{D}, X_*; \boldsymbol{\eta})$, often short as $p(\mathbf{y}_* | \mathbf{y})$.

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- The joint distribution of the **training output \mathbf{y}** and **test output \mathbf{y}_*** can be derived as

$$\begin{bmatrix} \mathbf{y} \\ \mathbf{y}_* \end{bmatrix} \sim \mathcal{N} \left(\mathbf{0}, \begin{bmatrix} K(X, X) + \beta^{-1} \mathbf{I}_n & K(X, X_*) \\ K(X_*, X) & K(X_*, X_*) + \beta^{-1} \mathbf{I}_{n_*} \end{bmatrix} \right).$$

- Applying the conditional Gaussian results, we obtain:

$$p(\mathbf{y}_* | \mathbf{y}) \sim \mathcal{N} (\bar{\mathbf{m}}, \bar{V}),$$

where

$$\bar{\mathbf{m}} \triangleq K(X_*, X) [K(X, X) + \beta^{-1} I_n]^{-1} \mathbf{y},$$

$$\begin{aligned}\bar{V} &\triangleq K(X_*, X_*) + \beta^{-1} I_{n_*} \\ &- K(X_*, X) [K(X, X) + \beta^{-1} I_n]^{-1} K(X, X_*).\end{aligned}$$

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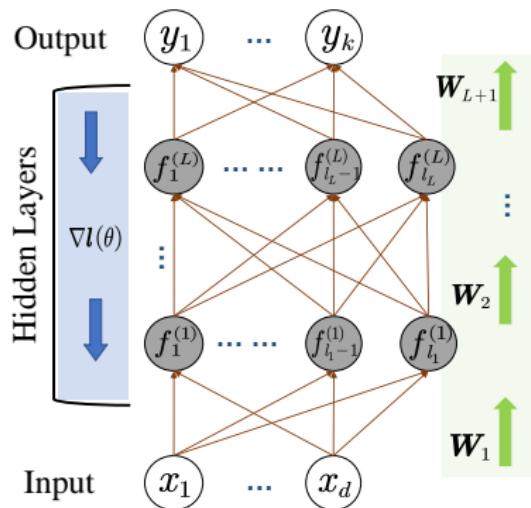
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Interpretations

- The posterior mean can be seen as a **linear predictor**.
- The posterior variance accounts the **difference** between **variance of the prior** and **variance explained by \mathcal{D}** .
- When using **linear kernel** the above results boil down to **Bayesian linear regression**.

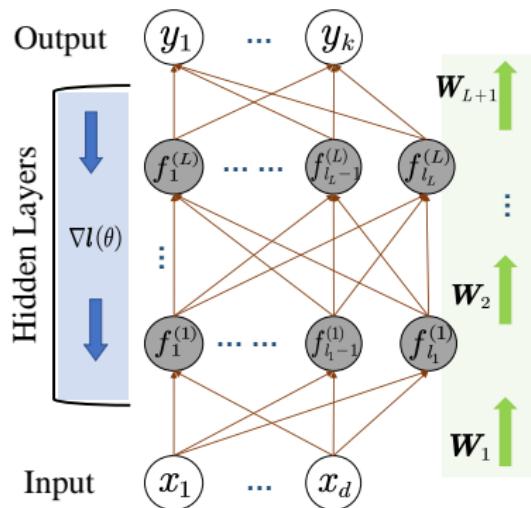
Connections between GP and NNs



- Each hidden layer comprises a large number of **nonlinear activation functions** to mimic the role of neurons in our brain.

¹K. Hornik, "Approximation capabilities of multilayer feedforward networks", *Neural Networks*, 1991.

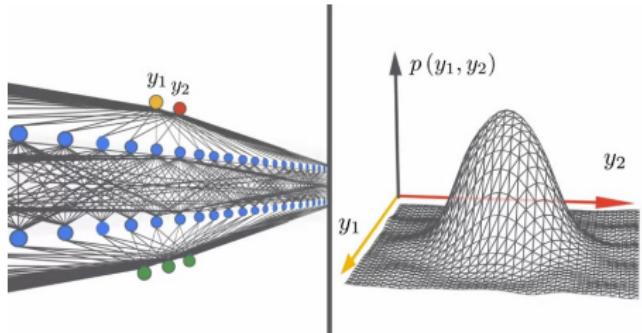
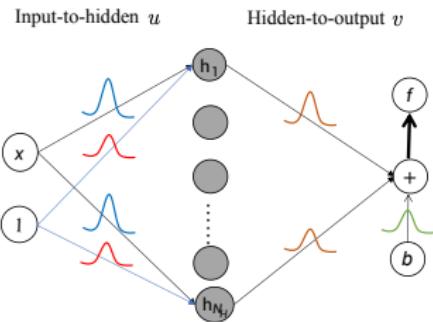
Connections between GP and NNs



- Each hidden layer comprises a large number of **nonlinear activation functions** to mimic the role of neurons in our brain.
- Neural network (NN) can approximate any smooth function arbitrarily well according to the **universal approximation theorem** [Hornik'91].¹

¹K. Hornik, "Approximation capabilities of multilayer feedforward networks", *Neural Networks*, 1991.

Connections between GP and NNs

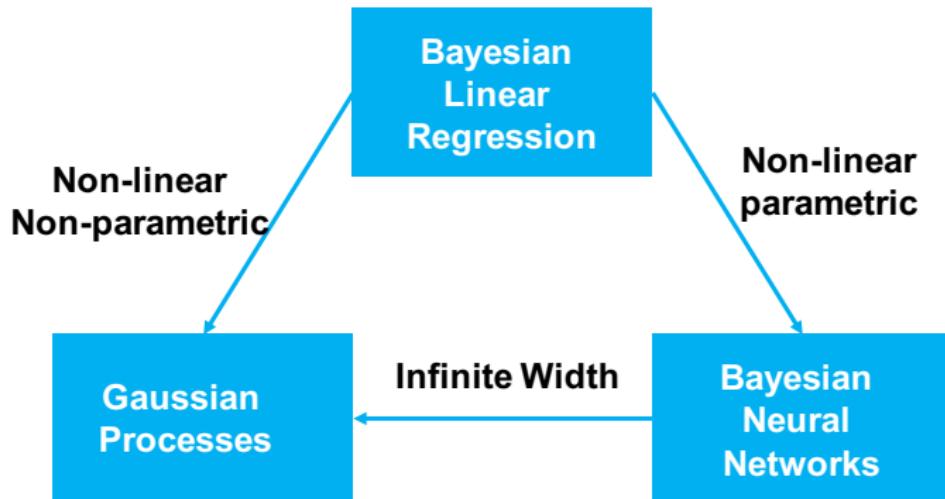


- GP and single layer NN
[MacKay'98] 2
- Neural network kernel
- GP and infinitely wide DNN
[Lee'18] 3
- Neural tangent kernel

²D. MacKay, "Introduction to Gaussian processes", *NATO ASI series F computer and systems sciences*, 1998.

³J. Lee, et al., "Deep neural networks as Gaussian processes", *ICLR*, 2018.

Section Conclusion



Outline

- 1 Motivation of Sparsity-Aware Learning
- 2 Sparsity-Aware Learning: from Frequentist to Bayesian
- 3 Sparsity-Aware Gaussian Process Models
- 4 Sparsity-Aware Bayesian Neural Network Models
- 5 Sparsity-Aware Tensor Decomposition Models
- 6 Applications of Modern Sparsity-Aware Models
- 7 Conclusion and Future Directions

Section Goals

This section aims to

- show a family of **interpretable and sparsity-promoting kernel prior** for nonparametric GP model;
- show the **kernel hyperparameter optimization process** and its benefits;
- explain the **sparsity-aware property** among other valuable ones.

Linear Multiple Kernel Design

- We focus on the **big family of linear multiple kernels**:

$$k(\mathbf{x}, \mathbf{x}') = \sum_{i=1}^Q \alpha_i k_i(\mathbf{x}, \mathbf{x}'),$$

where the weights, $\alpha_i, i = 1, 2, \dots, Q$, need to be optimized.

- The number of subkernels, Q , is often set large to form an over-complete dictionary of basis.
- Identify the most effective basis subkernels.

- Kernel design can be conducted either in raw input domain or in frequency domain.
- Design in raw input domain by ensembling a number of elementary kernels \Rightarrow analysis-of-variance kernel family.
- Design in frequency domain \Rightarrow sparse spectrum kernel family.

Design in Frequency Domain

Lemma (of Bochner's Theorem)

For 1-D time series where $x = t$, $\tau = t - t'$, its stationary kernel function, $k(\tau)$, and the spectral density, $S(\omega)$, form a Fourier pair:

$$k(\tau) = \int_{\mathbb{R}^1} S(f) \exp [j2\pi\tau\omega] df,$$
$$S(\omega) = \int_{\mathbb{R}^1} k(\tau) \exp [-j2\pi\tau\omega] d\tau.$$

Note: for simplicity, we let t represent time and ω represent normalized frequency.

First Sparse Spectrum (SS) Kernel

- Inspired by Bayesian linear regression with an over-complete set of trigonometric basis functions, $\{\cos(2\pi\omega_i x), \sin(2\pi\omega_i x)\}_{i=1}^Q$.⁴
- Feature mapping vector $\phi(x)$ contains all Q basis functions.

⁴ M. Lázaro-Gredilla, J. Quinonero Candela, C. E. Rasmussen, and A. R. Figueiras-Vidal, "Sparse spectrum Gaussian process regression," *J. Mach. Learn. Res.*, vol. 11, pp. 1865-1881, Aug. 2010.

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- Feature mapping vector $\phi(x)$ contains all Q basis functions.
- Choosing the weights to follow i.i.d. zero mean Gaussian, $\mathcal{N}(0, \frac{\sigma_0^2}{Q})$, the equivalent kernel function:

$$k(x, x') = \frac{\sigma_0^2}{Q} \phi^T(x) \phi(x') = \frac{\sigma_0^2}{Q} \sum_{i=1}^Q \cos(2\pi\omega_i(x - x')).$$

- The kernel hyperparameters, $\eta_p = [\sigma_0, \omega_1, \omega_2, \dots, \omega_Q]^T$, are to be optimized.

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Spectral Mixture Kernel: Frequency Domain

- Wilson et.al. proposed Spectral Mixture (SM) kernel⁵ to approximate the spectral density of the underlying kernel:

$$S(\omega) = \frac{1}{2} \sum_{i=1}^Q \frac{\alpha_i}{\sqrt{2\pi\sigma_i^2}} \left\{ \exp \left[\frac{-(\omega - \mu_i)^2}{2\sigma_i^2} \right] + \exp \left[\frac{-(\omega + \mu_i)^2}{2\sigma_i^2} \right] \right\}$$

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- Q is a preselected large number; α_i , μ_i , σ_i^2 are the weight, mean (center frequency) and variance of the i -th mixture component.

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SM Kernel: Raw Input Domain

- Taking the inverse Fourier transform of $S(\omega)$ yields a stationary kernel in the original input domain as

$$k(t, t'; \boldsymbol{\eta}_p) = k(\tau) = \sum_{i=1}^m \underbrace{\alpha_i \exp[-2\pi^2 \tau^2 \sigma_i^2] \cos(2\pi \tau \mu_i)}_{k_i(\tau)}$$

- The kernel hyperparameters $\boldsymbol{\eta}_p = [\alpha_1, \mu_1, \sigma_1, \dots, \alpha_Q, \mu_Q, \sigma_Q]^T$ are to be optimized.

SM Kernel: Approximation Capacity

- Approximate any stationary kernel arbitrary well in L_1 norm.

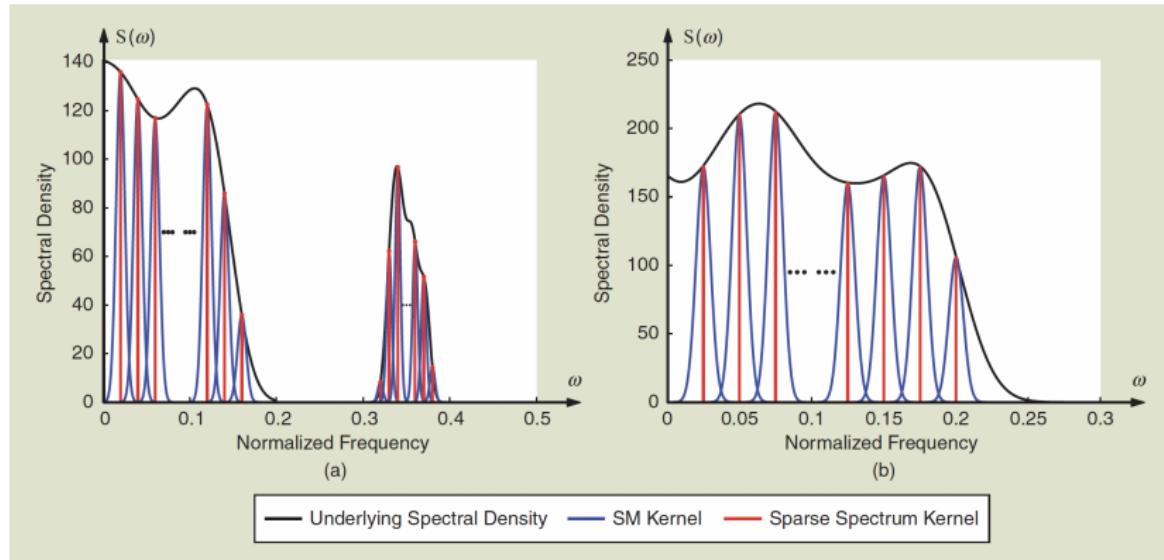
Theorem

For any stationary kernel $\tilde{k}(\tau)$ and an arbitrary $\epsilon > 0$, there exists Q_ϵ and for $m > Q_\epsilon$,

$$\int_{-\infty}^{\infty} \left| \sum_{i=1}^m \alpha_i \exp[-2\pi^2\tau^2\sigma_i^2] \cos(2\pi\tau\mu_i) - \tilde{k}(\tau) \right| d\tau < \epsilon.$$

Proof: Based on Wiener's theorem of approximation.

SS Kernel vs. SM Kernel



- SM kernel employs a **mixture of Gaussian basis functions** (blue curves)
- SS kernel employs a **mixture of Dirac deltas** (red vertical lines)

Numerical Difficulties of SS and SM Kernels

- It is generally difficult to tune the hyper-parameters due to **large-scale non-convex** optimization problem.
- Slower convergence and rather high probability of hitting **bad local minimum**.
- Relatively **high computational time** for big dataset.

Grid SM (GSM) Kernel

- To obtain nicer optimization structure, fix the mean and variance parameters to preselected grids, yielding the GSM kernel⁶:

$$k(t, t'; \eta_p) = k(\tau) = \sum_{i=1}^m \alpha_i \underbrace{\exp[-2\pi^2 \tau^2 \sigma_i^2] \cos(2\pi \tau \mu_i)}_{k_i(\tau)}$$

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- $k_i(\tau)$ can be seen as a fixed sub-kernel without any hyper-parameters to be tuned.
- The kernel hyperparameters $\eta_p = \alpha \triangleq [\alpha_1, \alpha_2, \dots, \alpha_m]^T \geq \mathbf{0}$ are to be optimized.

GSM kernel is essentially a linear multiple kernel!

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Inference Algorithms for GP with GSM Kernel

- Evidence is mathematically tractable for GP model.
- Maximizing the evidence is equivalent to

$$\begin{aligned}\hat{\boldsymbol{\eta}}_{ML} = \arg \min_{\boldsymbol{\eta}=\{\boldsymbol{\alpha}, \sigma_e^2\}} \ell(\boldsymbol{\eta}) &\triangleq \mathbf{y}^T \mathbf{C}^{-1}(\boldsymbol{\alpha}, \sigma_e^2) \mathbf{y} + \log \det (\mathbf{C}(\boldsymbol{\alpha}, \sigma_e^2)) \\ \text{s.t. } \boldsymbol{\alpha} &\geq \mathbf{0}, \sigma_e^2 \geq 0.\end{aligned}$$

- $\mathbf{C}(\boldsymbol{\alpha}, \sigma_e^2) \triangleq \sum_{i=1}^Q \boldsymbol{\alpha}_i \mathbf{K}_i + \sigma_e^2 \mathbf{I}_n$ is the overall covariance matrix including the noise term.

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- $\mathbf{C}(\boldsymbol{\alpha}, \sigma_e^2) \triangleq \sum_{i=1}^Q \boldsymbol{\alpha}_i \mathbf{K}_i + \sigma_e^2 \mathbf{I}_n$ is the overall covariance matrix including the noise term.
- Let $g(\boldsymbol{\eta}) \triangleq \mathbf{y}^T \mathbf{C}^{-1}(\boldsymbol{\alpha}, \sigma_e^2) \mathbf{y}$ and $h(\boldsymbol{\eta}) \triangleq -\log \det (\mathbf{C}(\boldsymbol{\alpha}, \sigma_e^2)).$
- The above is provably a difference-of-convex (DCP) problem.

- An effective way to handle DCP is via the majorization-minimization (MM) algorithm.

- An effective way to handle DCP is via the **majorization-minimization (MM) algorithm**.
- Introduce a so-called **majorization function** $\bar{\ell}(\eta, \eta^k)$ of $\ell(\eta)$ at $\eta^k \in \Theta$ and solve instead

$$\eta^{k+1} = \arg \min_{\eta \in \Theta} \bar{\ell}(\eta, \eta^k),$$

where $\bar{\ell} : \Theta \times \Theta \rightarrow \mathbb{R}$ satisfies:

- ① $\bar{\ell}(\eta, \eta) = \ell(\eta)$ for $\eta \in \Theta$,
- ② and $\ell(\eta) \leq \bar{\ell}(\eta, \eta')$ for $\eta, \eta' \in \Theta$.

- Adopting the simple linear majorization to make the convex function $h(\theta)$ affine by performing first-order Taylor expansion.
- Consequently, $\bar{I}(\theta, \theta^k) \triangleq g(\theta) - h(\theta^k) - \nabla_{\theta}^T h(\theta^k)(\theta - \theta^k)$.

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- We also developed an ADMM algorithm that has the same computational complexity.

Rationale behind Sparsity Awareness

- Treat the overall GP model as a sum of Q independent GP models.
- Each subkernel $k_i(\mathbf{x}, \mathbf{x}') = \phi_i^T(\mathbf{x})\phi_i(\mathbf{x}')$, where $\phi_i(\mathbf{x}) : \mathbb{R}^L \mapsto \mathbb{R}^{L'}$, with $L' \gg L$.
- Then, $f(\mathbf{x}) = \sum_{i=1}^Q \boldsymbol{\theta}_i^T \phi_i(\mathbf{x})$, where $\boldsymbol{\theta}_i \sim \mathcal{N}(\mathbf{0}, \alpha_i \mathbf{I})$.

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- Mathematical proof follows the sparsity-promoting property of the *relevance vector machine* for classic sparse linear model.⁷
- Maximizing the evidence is equivalent to finding the most relevant basis vectors in the over-complete dictionary, $\{\phi_i\}_{i=1}^Q$.

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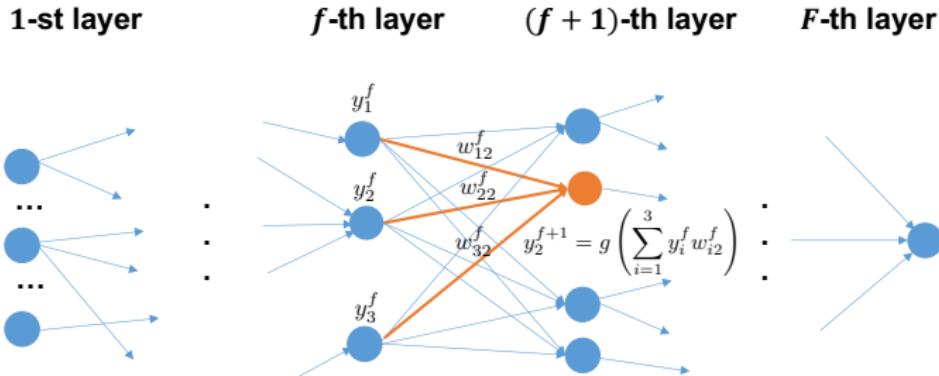
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Section Goals

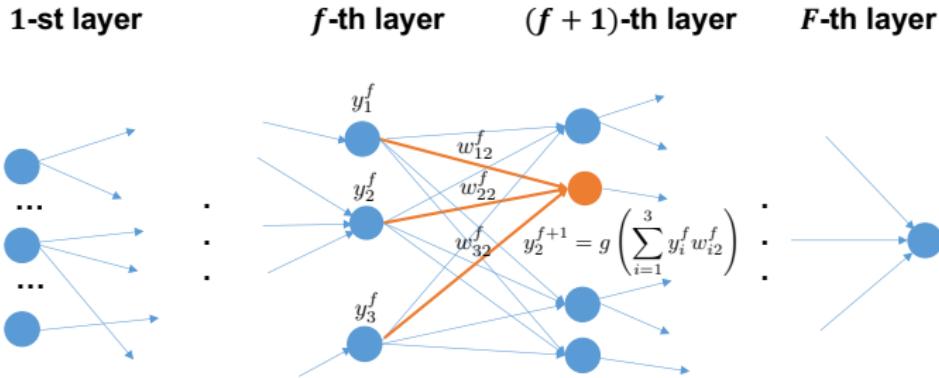
- We introduce **sparsity-promoting techniques** for **pruning** Bayesian deep neural networks (DNNs).
- That is, starting from a neural network with **enormous number of nodes**, to optimally **remove** nodes and/or links.
- We are going to follow two paths:
 - ① **Path 1:** The **parametric** one via the Gaussian Scale Mixture (GSM) priors;
 - ② **Path 2:** The **non-parametric** one via the Indian Buffet Process (IBP) prior.

Revisit Fundamentals of DNN



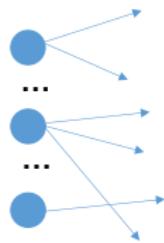
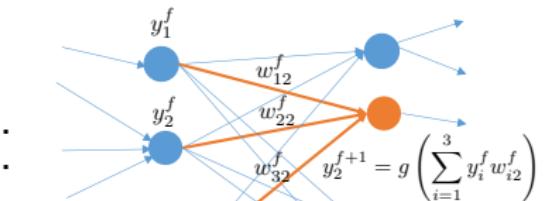
- Consider a fully connected DNN consisting of F layers.

Revisit Fundamentals of DNN



- Consider a fully connected DNN consisting of F layers.
- The number of nodes in the f -th ($1 \leq f \leq F - 1$) layer is a^f .
- For the i -th node in the f -th layer and the j -th node in the $(f + 1)$ -th layer, the link between them has a weight w_{ij}^f .

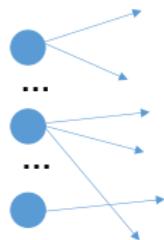
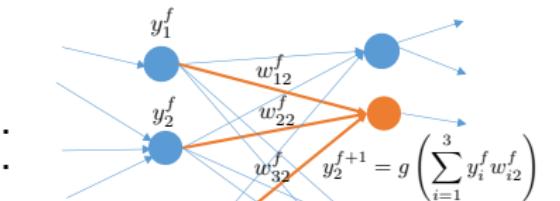
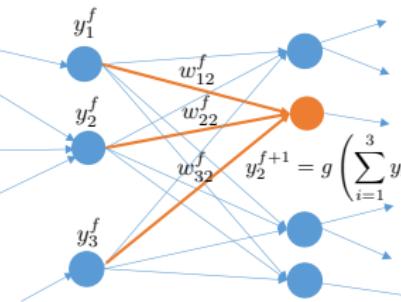
1-st layer

 f -th layer $(f + 1)$ -th layer F -th layer

- The input vector to the $(f + 1)$ -th layer: $\mathbf{y}^f = [y_1^f, y_2^f, \dots, y_{a^f}^f]^T$.
- The link weights associated with the j -th node:

$$\mathbf{w}_j^f = [w_{1j}^f, w_{2j}^f, \dots, w_{a^f j}^f]^T.$$

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- The link weights associated with the j -th node:

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- The output of the j -th node is:

$$y_j^{f+1} = g\left(\sum_{i=1}^{a^f} w_{ij}^f y_i^f\right) = g\left(\left[\mathbf{w}_j^f\right]^T \mathbf{y}^f\right),$$

where $g(\cdot)$ is a **nonlinear activation function**.

Sparsity-Aware Modeling Using GSM Priors

- The idea dates back to the pioneering work of D. J. MacKay.⁸
- NN with **a single hidden layer**, the link weights can be treated as *random variables*.

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- This induces an “inductive bias” of being sparse to the network.

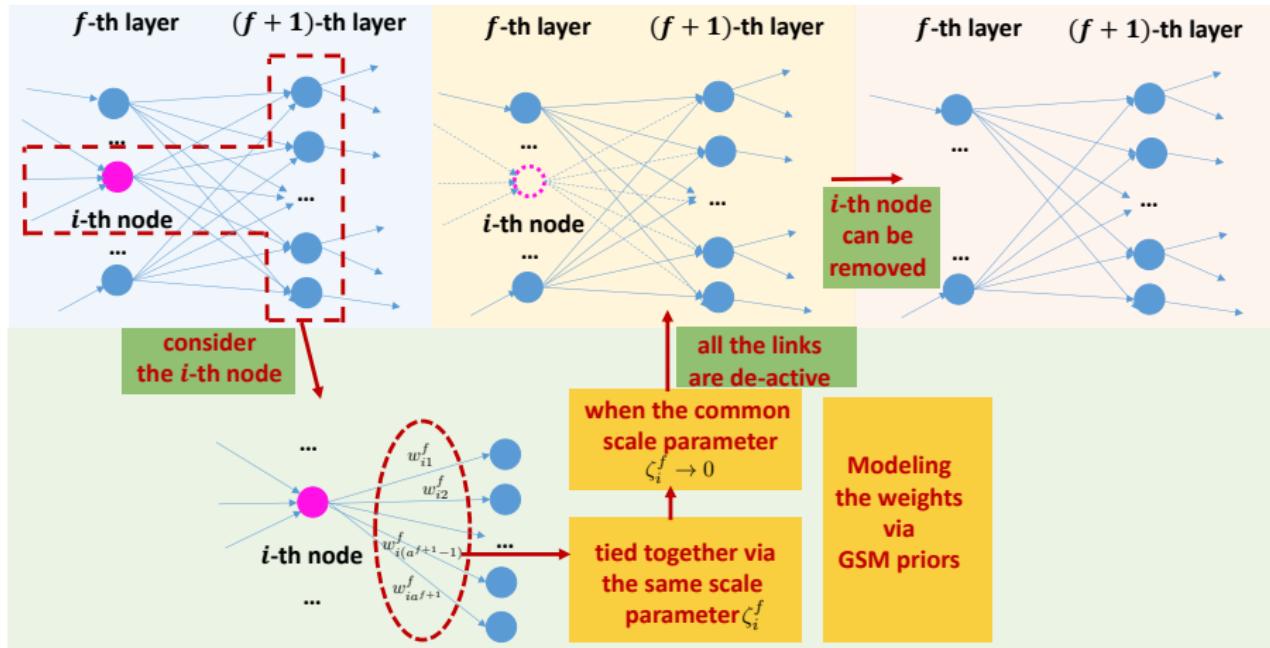
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- This induces an “inductive bias” of being sparse to the network.
- The major difference between recent works and early ones lies in the adopted priors.

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- Global picture of node-wise sparsity rationale.



- For each random weight w_{ij}^f , we adopt a sparsity-promoting GSM prior:

$$p(w_{ij}^f) = \int \mathcal{N}(w_{ij}^f; 0, \zeta_{ij}^f) p(\zeta_{ij}^f; \boldsymbol{\eta}) d\zeta_{ij}^f.$$

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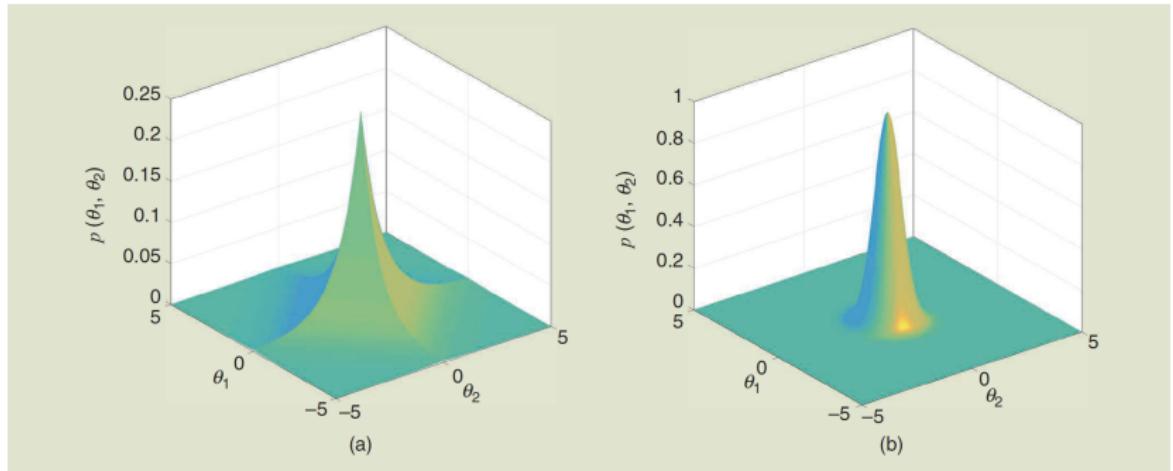
- Functional form of $p(\zeta_{ij}^f; \boldsymbol{\eta})$ below corresponds to a GSM prior.

GSM prior $p(w_I)$	Mixing distribution $p(\zeta_I)$
Student's t	Inverse Gamma: $p(\zeta_I; \boldsymbol{\eta}_p = [a, b]) = \text{IG}(\zeta_I; a, b)$
Normal-Jefferys	Log-uniform: $p(\zeta_I; \boldsymbol{\eta}_p = []) \propto \frac{1}{ \zeta_I }$
Laplacian	Gamma: $p(\zeta_I; \boldsymbol{\eta}_p = [a, b]) = \text{Ga}(\zeta_I; a, b)$
Generalized hyperbolic	Generalized inverse Gaussian: $p(\zeta_I; \boldsymbol{\eta}_p = [a, b, \lambda]) = \text{GIG}(\zeta_I; a, b, \lambda)$
Horseshoe	$\zeta_I = \tau_I v_I, \boldsymbol{\eta}_p = [a, b]$ Half Cauchy: $p(\tau_I) = C^+(0, a)$ $p(v_I) = C^+(0, b)$

- Next, we show how to conduct node-wise sparsity-aware modeling.
- Group the weights $\{w_{ij}^f\}_{j=1}^{a^{f+1}}$ connected to the i -th node, and assign a common scale parameter ζ_i^f to their GSM priors, i.e., $\zeta_{ij}^f = \zeta_i^f, \forall j$.

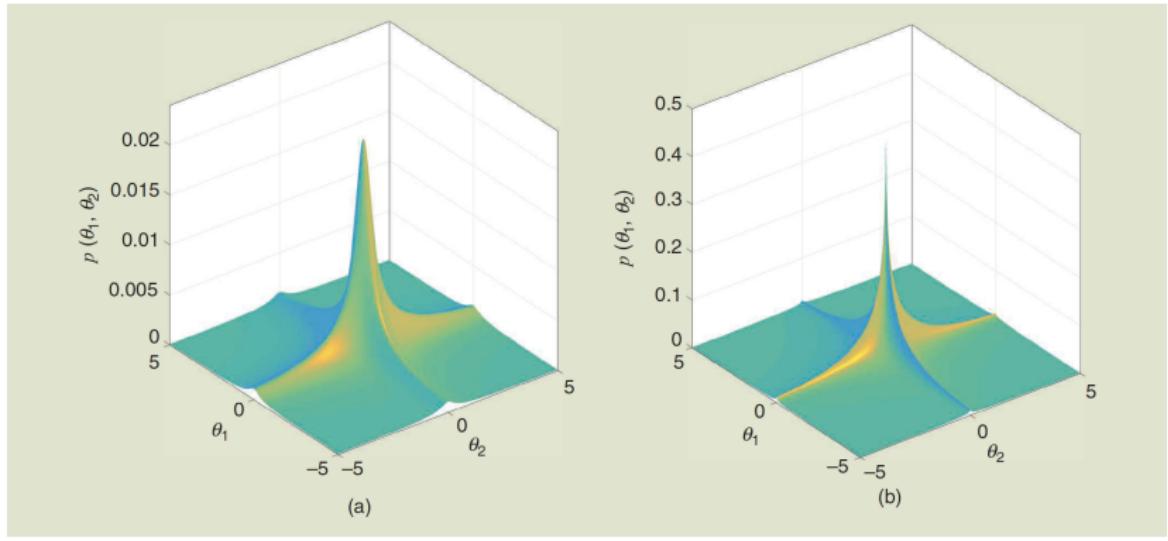
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- The prior modeling for the i -th node related weights $\{w_{ij}^f\}_{j=1}^{a^{f+1}}$:

$$\begin{aligned} p(\{w_{ij}^f\}_{j=1}^{a^{f+1}}) &= \int p(\{w_{ij}^f\}_{j=1}^{a^{f+1}} | \zeta_i^f) p(\zeta_i^f; \boldsymbol{\eta}) d\zeta_i^f \\ &= \int \prod_{j=1}^{a^{f+1}} \mathcal{N}(w_{ij}^f; 0, \zeta_i^f) p(\zeta_i^f; \boldsymbol{\eta}) d\zeta_i^f. \end{aligned}$$



The joint probability distribution of the model parameters in 2D space. (a) The Laplacian distribution. (b) The Gaussian distribution.

- Heavy-tail Laplacian distribution peaks sharply around zero and falls slowly along the axes, thus promoting sparse solutions.
- Gaussian distribution decays more rapidly along both dimensions when compared to the Laplacian distribution.



(a) The Student's t distribution versus (b) the horseshoe distribution.

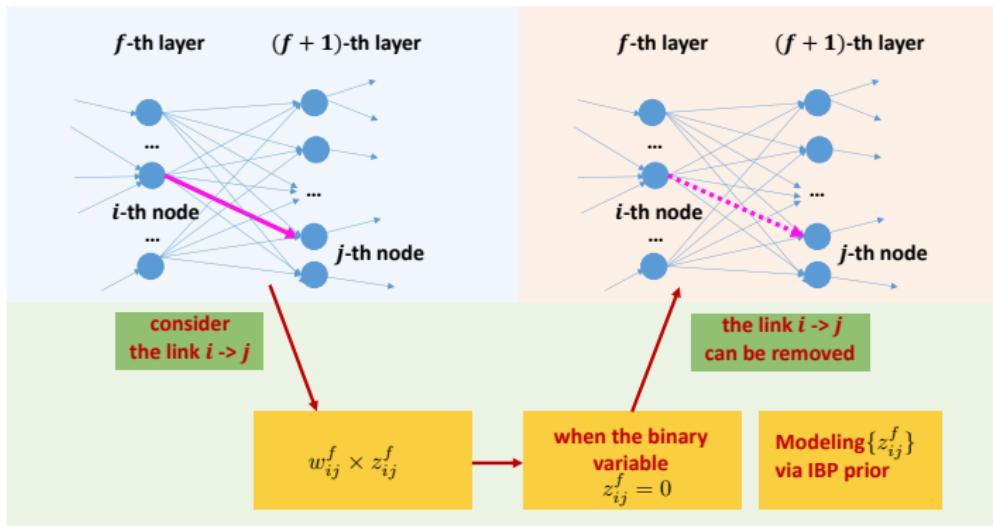
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Sparsity-Aware Modeling Using IBP Prior

- The previous approach has a major drawback, i.e., the number of nodes per layer has to be specified and pre-selected.
- In contrast, we now turn our attention to non-parametric techniques for link-wise sparsity.
- We are going to assume that the nodes per layer are theoretically infinite (in practice a large enough number) and then use the IBP prior to enforce sparsity.

- Global picture of the rationale behind link-wise sparsity-aware modeling.



- We multiply each weight, i.e., w_{ij}^f , with a corresponding auxiliary (hidden) binary random variable, z_{ij}^f .

Brief Introduction to IBP Prior

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- Assuming an Indian restaurant offers $K \rightarrow \infty$ of dishes ([output dimension](#)) and there are L customers ([input dimension](#)).

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- Rationale of IBP:
 - ① The first dimension, say, x_1 is linked to some of the infinite nodes with certain probabilities;
 - ② The second dimension, x_2 is linked to some of the previously linked nodes and to some new ones according to certain probabilities;
 - ③ ... until x_L .

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 - ② The second dimension, x_2 is linked to some of the previously linked nodes and to some new ones according to certain probabilities;
 - ③ ... until x_L .
- Mathematically, we aim to generate **a series of binary random variables**, $z_{ij} \in \{0, 1\}$, $i = 1, 2, \dots, L$ and $j = 1, 2, \dots$
- If $z_{ij} = 1$, the i -th customer (i -th dimension) selects the j -th dish (linked to the j -th node).

- Following the stick-breaking construction idea, first generate:

$$u_j \sim \text{Beta}(u_j|\alpha, 1), \quad \pi_j = \prod_{l=1}^j u_l, \quad j = 1, 2, \dots.$$

- Then, the generated probabilities, π_j , are used to populate the matrix Z , by drawing samples from a Bernoulli distribution:

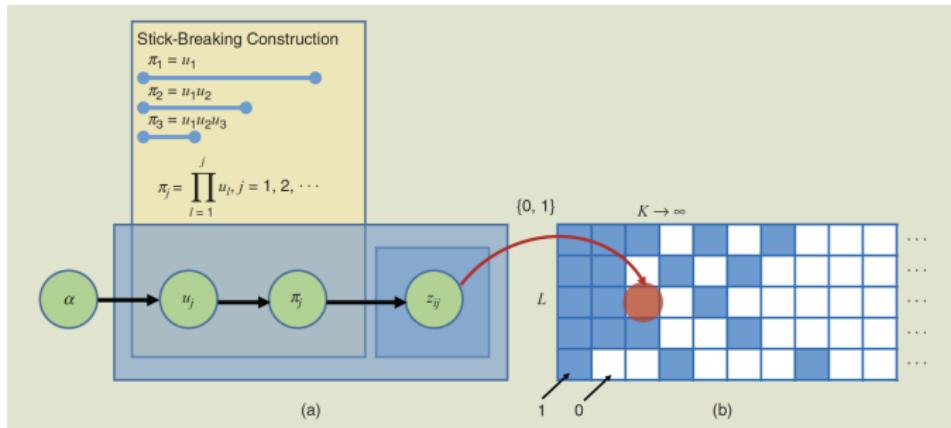
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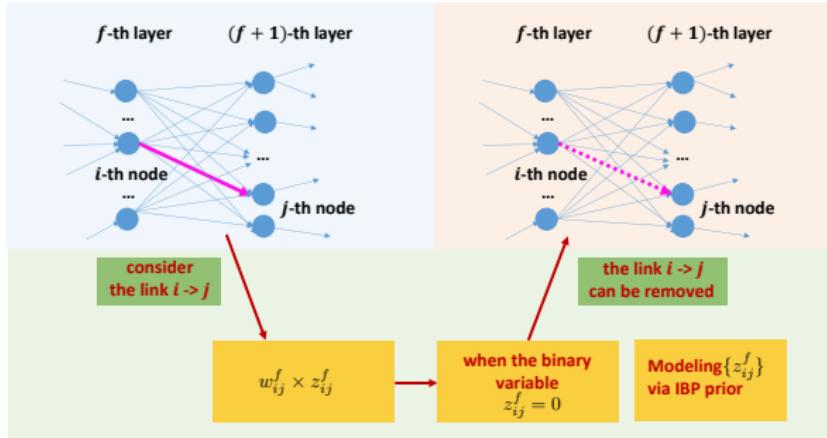
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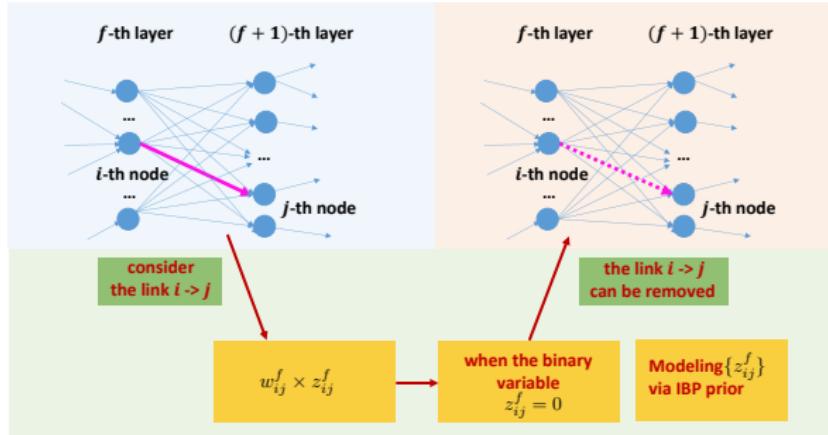
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(a):Beta-Bernoulli model. (b): The binary matrix Z .





- $\{\{z_{ij}^f\}_{i=1}^{a^f}\}_{j=1}^{a^{f+1}}$ are generated via the stick-breaking IBP prior:

$$u_j^f \sim \text{Beta}(u_j^f | \alpha, 1), \quad \pi_j^f = \prod_{l=1}^j u_l^f, \quad z_{ij}^f \sim \text{Bernoulli}(z_{ij}^f | \pi_j^f).$$

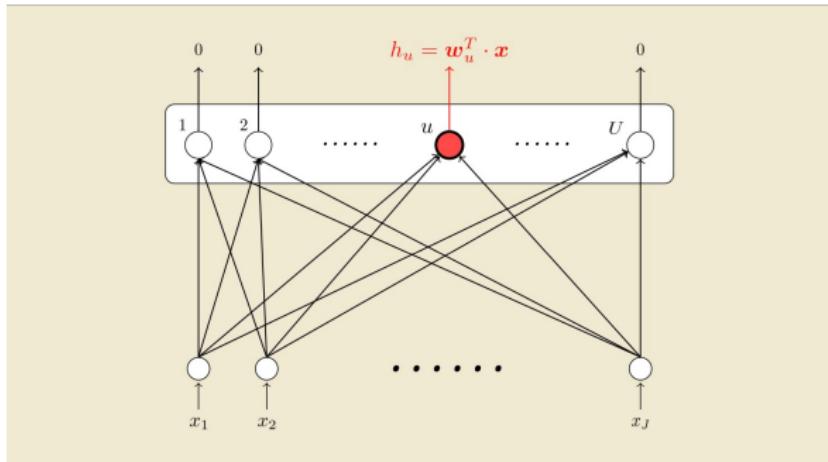
- Binary matrix $\mathbf{Z}^f \in \mathbb{R}^{a^f \times a^{f+1}}$, with its (ij) -th element being z_{ij}^f for the f -th layer.

- The flexibility of the link-wise formulation allows us to go one step further.
- Recently, the stick-breaking IBP prior was combined with a radically different, biologically-inspired and competition-based activation, namely the stochastic local winner-takes-all (LWTA).^{9, 10, 11}
- LWTA adopts blocks of competing linear units/neurons against ordinary neurons with nonlinear activation for nonlinearity.

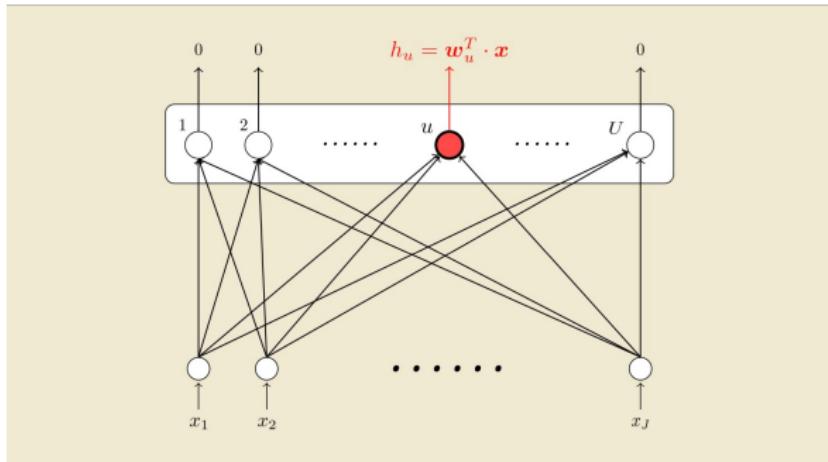
⁹ K. Panousis, S. Chatzis, and S. Theodoridis, "Nonparametric Bayesian deep networks with local competition," in ICML, 2019.

¹⁰ K. Panousis, S. Chatzis, A. Alexos, and S. Theodoridis, "Local competition and stochasticity for adversarial robustness in deep learning," in AISTAT, 2021.

¹¹ K. Panousis, S. Chatzis, and S. Theodoridis, "Stochastic local winner-takes-all networks enable profound adversarial robustness," in NeurIPS, 2021.

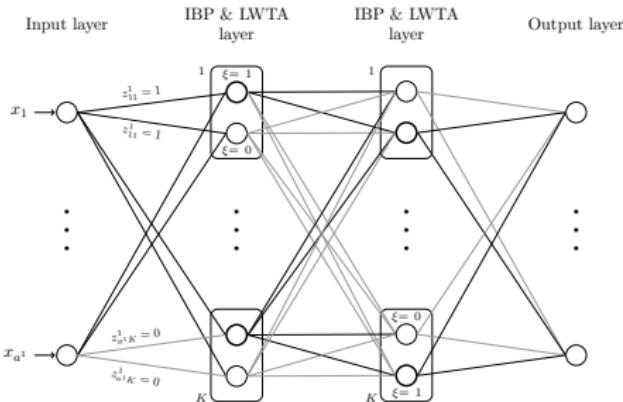


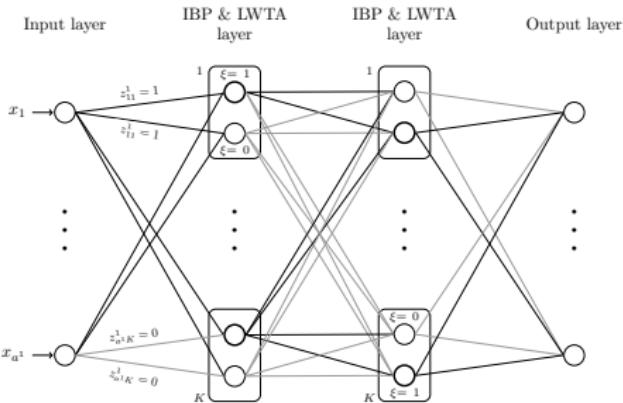
- Each node comprises a set of linear (inner product) units.



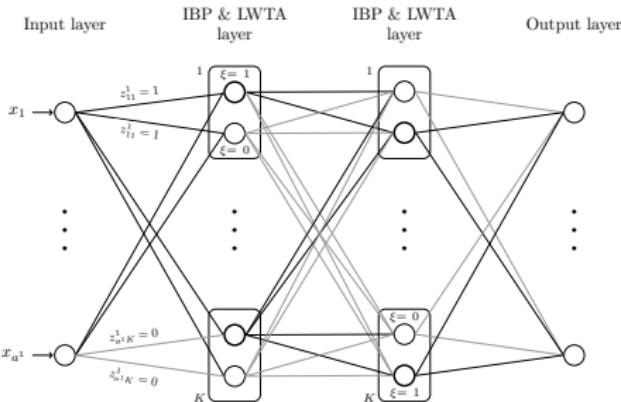
- Each node comprises a set of linear (inner product) units.
- The unit with the *strongest* activation is deemed to be the *winner* and passes its output to the next layer, while the rest are being zero.
- This deterministic winner selection is known as *hard* LWTA.
- We turn to *stochastic LWTA* with enhanced performance.

- L inputs, K LWTA blocks; J linear units.
- Here, $L = a^1$, $J = 2$ for each layer.





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- z_{ik} is modeled by IBP as introduced before.
- Weights:
 $w_{ikj}, i = 1, 2, \dots, L, k = 1, 2, \dots, K, j = 1, 2, \dots, J.$

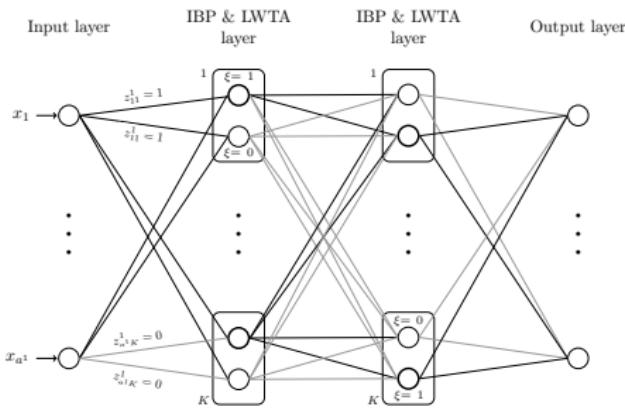


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Linear unit output is:

$$y_{kj} = \xi_{kj} \mathbf{w}_{kj}^T \mathbf{x} = \xi_{kj} \sum_{i=1}^L w_{ikj} x_i, \quad \xi_{kj} \in \{0, 1\}, \quad \sum_{j=1}^J \xi_{kj} = 1.$$

- The output depends on the value of $\xi_{kj} \in \{0, 1\}$.
- The respective probabilities, which control the value of ξ_{kj} , are computed via *softmax*:



$$P_{kj} = \frac{\exp(h_{kj})}{\sum_{j=1}^J \exp(h_{kj})},$$

$$h_{kj} = \sum_{i=1}^L (\textcolor{blue}{z}_{ik} w_{ikj}) x_i.$$

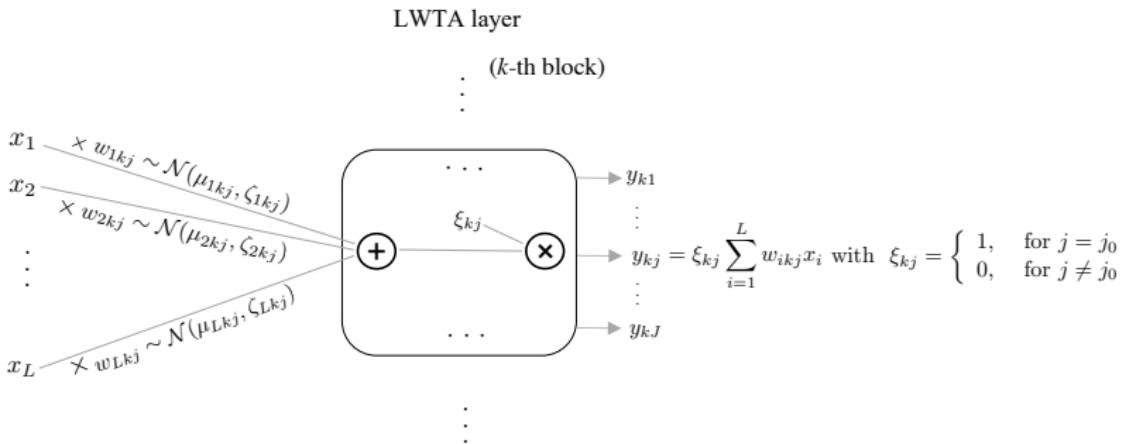
Inference Algorithms for Bayesian DNNs

- Inference (training) for Bayesian deep neural networks follows the same **backpropagation-type** of philosophy as that of deterministic DNNs.

Inference Algorithms for Bayesian DNNs

- Inference (training) for Bayesian deep neural networks follows the same backpropagation-type of philosophy as that of deterministic DNNs.
- There are, however, two notable differences:
 - First, the unknown (synaptic) parameters/weights are now described via parameterized distributions.
 - Second, the evidence function to be maximized is intractable and has to be approximated by its ELBO.

- We focus on the Bayesian deep network that comprises layers with:
 - stochastic LWTA blocks;
 - stochastic synaptic weights of Gaussian form;
 - a sparsity-inducing mechanism imposed over the network synapses that is driven via an IBP prior.



■ Synaptic weights:

Prior : $p(w_{ikj}) \sim \mathcal{N}(w_{ikj}|0, 1)$, Posterior : $q(w_{ikj}) \sim \mathcal{N}(w_{ikj}|\mu_{ikj}, \zeta_{ikj})$

■ Utility binary random variables:

Prior : Beta($u_k|\alpha, 1$), Posterior : $q(u_k) = \text{Beta}(u_k|a_k, b_k)$

Prior : Bernoulli($z_{ik}|\pi_{ik}$), Posterior : $q(z_{ik}) = \text{Bernoulli}(z_{ik}|\tilde{\pi}_{ik})$

■ Indicator random vectors, ξ_k :

Prior : $p(\xi_k) = \text{Categorical}(\xi_k|\frac{1}{J}, \dots, \frac{1}{J})$, i.e., all linear units equiprobable.

Posterior : $q(\xi_k) = \text{Categorical}(\xi_k|P_{k1}, \dots, P_{kJ})$

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- The hyperparameters to be optimized include:

$$\boldsymbol{\theta} = [\{\mu_{ikj}\}, \{\zeta_{ikj}\}, \{a_k\}, \{b_k\}, \{\tilde{\pi}_{ik}\}].$$

- \mathcal{D} : input-output training dataset;
- \mathbf{Z} : set of the synaptic utility indicators across the network layers;
- $\mathbf{\Xi}$: set of winner unit indicators across all blocks of all layers;
- \mathbf{W} : set of synapse weights across all layers;
- \mathbf{U} : set of the stick-variables of the sparsity-inducing priors imposed across the network layers.

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 - \mathbf{U} : set of the stick-variables of the sparsity-inducing priors imposed across the network layers.
- Employing the mean-field approximation $q(\mathbf{W}, \mathbf{Z}, \Xi, \mathbf{U})$ to obtain:

$$\text{ELBO}(\theta) = \mathbb{E}_q \left[\sum_{n=1}^N \sum_{c=1}^C y_{nc} \ln \tilde{y}_{nc}(\mathbf{x}_n; \mathbf{W}, \mathbf{Z}, \Xi, \mathbf{U}) \right]$$

$$+ \underbrace{\mathbb{E}_q \ln \frac{p(\mathbf{Z}|\mathbf{U})}{q(\mathbf{Z})} + \mathbb{E}_q \ln \frac{p(\mathbf{U})}{q(\mathbf{U})}}_{\text{regularizing terms}} + \underbrace{\mathbb{E}_q \ln \frac{p(\Xi)}{q(\Xi|\mathbf{Z}, \mathbf{W})} + \mathbb{E}_q \ln \frac{p(\mathbf{W})}{q(\mathbf{W})}}_{\text{regularizing terms}}$$

- To approximate the expectations in ELBO via samples, we introduce **reparameterization trick**.

Example: Let $\mathcal{N}(w_{ikj} | \mu_{ikj}, \zeta_{ikj})$ be the current estimate. We have

$$\tilde{w}_{ikj} = \mu_{ikj} + \zeta_{ikj}^{1/2} \cdot \epsilon, \quad \epsilon \sim \mathcal{N}(0, 1).$$

- In this way, **every link is determined explicitly by the pair (μ_{ijk}, ζ_{ijk})** ; and the backpropagation optimizes the means and variances.
- Reparameterization of the rest variables **follows a similar rationale**.

⁹K. Panousis, S. Chatzis, and S. Theodoridis, "Nonparametric Bayesian deep networks with local competition," in ICML, 2019.

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- In this way, **every link is determined explicitly by the pair (μ_{ijk}, ζ_{ijk})** ; and the backpropagation optimizes the means and variances.
- Reparameterization of the rest variables **follows a similar rationale**.
- Off-the-shelf gradient-based optimizer**, e.g., the Adam, can be used for training.
- More details about the inference algorithm can be found here.⁹

⁹ K. Panousis, S. Chatzis, and S. Theodoridis, "Nonparametric Bayesian deep networks with local competition," in ICML, 2019.

Outline

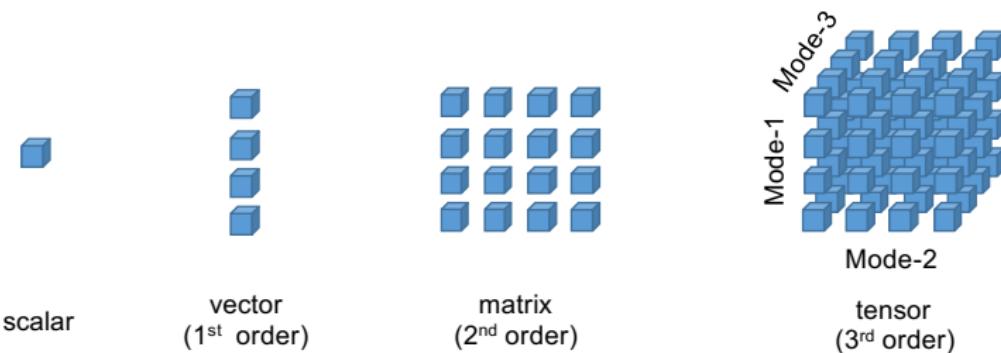
- 1 Motivation of Sparsity-Aware Learning
- 2 Sparsity-Aware Learning: from Frequentist to Bayesian
- 3 Sparsity-Aware Gaussian Process Models
- 4 Sparsity-Aware Bayesian Neural Network Models
- 5 Sparsity-Aware Tensor Decomposition Models
- 6 Applications of Modern Sparsity-Aware Models
- 7 Conclusion and Future Directions

Section Goals

- So far, we have elucidated the sparsity-aware learning for the two recent **supervised** data analysis tools, namely the DNNs and GPs.
- Their underlying idea has inspired recent study for the **unsupervised learning tools**, e.g., **tensor decomposition**.
- We take the most fundamental ***canonical polyadic decomposition (CPD)*** as an example to elucidate the key ideas of
 - Prior Modeling;
 - Inference Method.

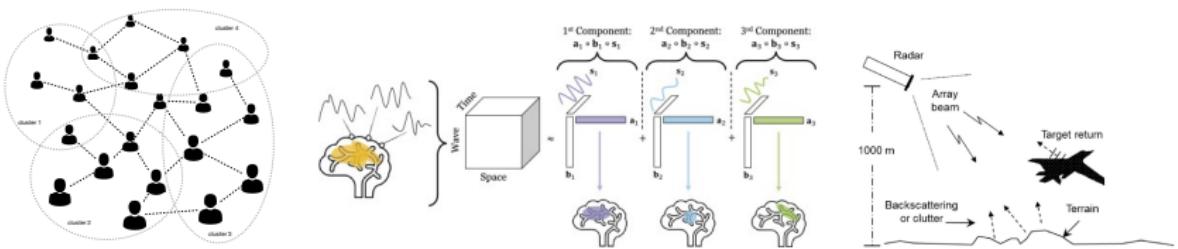
Tensors and CPD

- Tensors are regarded as multi-dimensional generalization of matrices.



- Specifically, a P -dimensional (P -D) dataset can be represented by a P -D tensor $\mathcal{D} \in \mathbb{R}^{J_1 \times J_2 \times \dots \times J_P}$.

- Given a tensor \mathcal{D} , unsupervised learning aims to **identify the underlying source signals** that generated the observed data:
 - “Clustering” in social network analysis
 - “Blind source separation” in EEG data analysis
 - “Blind signal estimation” in radar/sonar signal processing



Figures are from [12]-[13].

¹² S. Redif, S. Weiss, and J. G. McWhirter. Relevance of polynomial matrix decompositions to broadband blind signal separation. *Signal processing*, 134, 76-86, 2017.

¹³ <https://www.sciencedirect.com/topics/engineering/blind-signal-separation>

Tensor CPD has been proven to be a powerful tool with good interpretability. It is formally defined as follows¹⁴.

Definition of Tensor CPD

Given a P -D tensor $\mathcal{D} \in \mathbb{R}^{J_1 \times J_2 \times \dots \times J_P}$, CPD seeks to find the vectors $\{\mathbf{a}_r^{(1)}, \mathbf{a}_r^{(2)}, \dots, \mathbf{a}_r^{(P)}\}_{r=1}^R$ such that

$$\begin{aligned}\mathcal{D} &= \sum_{r=1}^R \underbrace{\mathbf{a}_r^{(1)} \circ \mathbf{a}_r^{(2)} \circ \dots \circ \mathbf{a}_r^{(P)}}_{\text{rank-1 tensor}}, \\ &\triangleq [\![\mathbf{A}^{(1)}, \mathbf{A}^{(2)}, \dots, \mathbf{A}^{(P)}]\!],\end{aligned}$$

where \circ denotes vector outer product; $\mathbf{A}^{(p)} \triangleq [\mathbf{a}_1^{(p)}, \mathbf{a}_2^{(p)}, \dots, \mathbf{a}_R^{(p)}] \in \mathbb{R}^{J_p \times R}, \forall p$, is called the factor matrix. The minimal number R that yields the above expression is termed as the tensor rank.

¹⁴ N. D. Sidiropoulos, L. De Lathauwer, X. Fu, K. Huang, E. E. Papalexakis and C. Faloutsos, "Tensor Decomposition for Signal Processing and Machine Learning," in IEEE Transactions on Signal Processing, vol. 65, no. 13, pp. 3551-3582, 2017. ↗ ↘ ↙ ↛ ↜

Inspect the definition of tensor CPD:

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- When $P = 2$, it reduces to decomposing a matrix $\mathbf{D} \in \mathbb{R}^{J_1 \times J_2}$ into the summation of R rank-1 matrices, i.e., $\mathbf{D} = \sum_{r=1}^R \mathbf{a}_r^{(1)} \circ \mathbf{a}_r^{(2)}$.

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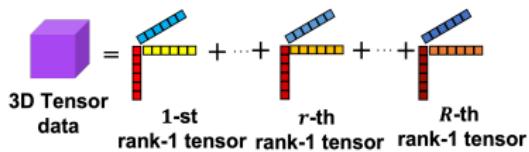
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- By defining the term $\mathbf{a}_r^{(1)} \circ \mathbf{a}_r^{(2)} \circ \cdots \circ \mathbf{a}_r^{(P)}$ as a P -D rank-1 tensor, CPD essentially seeks for R rank-1 tensors/components from the observed dataset.

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- Each rank-1 tensor corresponds to one specific underlying source signal.
- The tensor rank R has a clear physical meaning as the number of the underlying source signals.



Low-Rank CPD and Sparsity-Aware Modeling

- In real-world applications, the number of source signals is usually small.
- For instance, in brain-source imaging, the EEG data analysis has shown that only a small fraction of source signals contribute to the brain activities.

15

L. Cheng, Z. Chen, Y. -C. Wu and S. Theodoridis, "Towards Flexible Sparsity-Aware Modeling: Automatic Tensor Rank Learning Using the Generalized Hyperbolic Prior," IEEE Transactions on Signal Processing, vol. 70, pp. 1834-1849, 2022.



Low-Rank CPD and Sparsity-Aware Modeling

- In real-world applications, the number of source signals is usually small.
- For instance, in brain-source imaging, the EEG data analysis has shown that only a small fraction of source signals contribute to the brain activities.
- This suggests that the CPD model should assume a low tensor rank R to avoid data overfitting.
- In the sequel, we show how the *low-rankness* is probabilistically embedded into the CPD model through practicing the ideas reported previously¹⁵.

¹⁵ L. Cheng, Z. Chen, Y. -C. Wu and S. Theodoridis, "Towards Flexible Sparsity-Aware Modeling: Automatic Tensor Rank Learning Using the Generalized Hyperbolic Prior," IEEE Transactions on Signal Processing, vol. 70, pp. 1834-1849, 2022.

- We employ an over-parameterized model for CPD by assuming an upper-bound value L of tensor rank R , i.e., $L \gg R$.
- The low-rankness implies that $(L - R)$ rank-1 tensors should be zero, each specified by vectors $\{\mathbf{a}_I^{(p)}\}_{p=1}^P, \forall I$.
- Let vector $\mathbf{q}_I \triangleq [\mathbf{a}_I^{(1)}; \mathbf{a}_I^{(2)}; \dots; \mathbf{a}_I^{(P)}] \in \mathbb{R}^{\sum_{p=1}^P J_p}, \forall I$. The low-rankness indicates that a number of vectors in the set $\{\mathbf{q}_I\}_{I=1}^L$ are zero vectors.

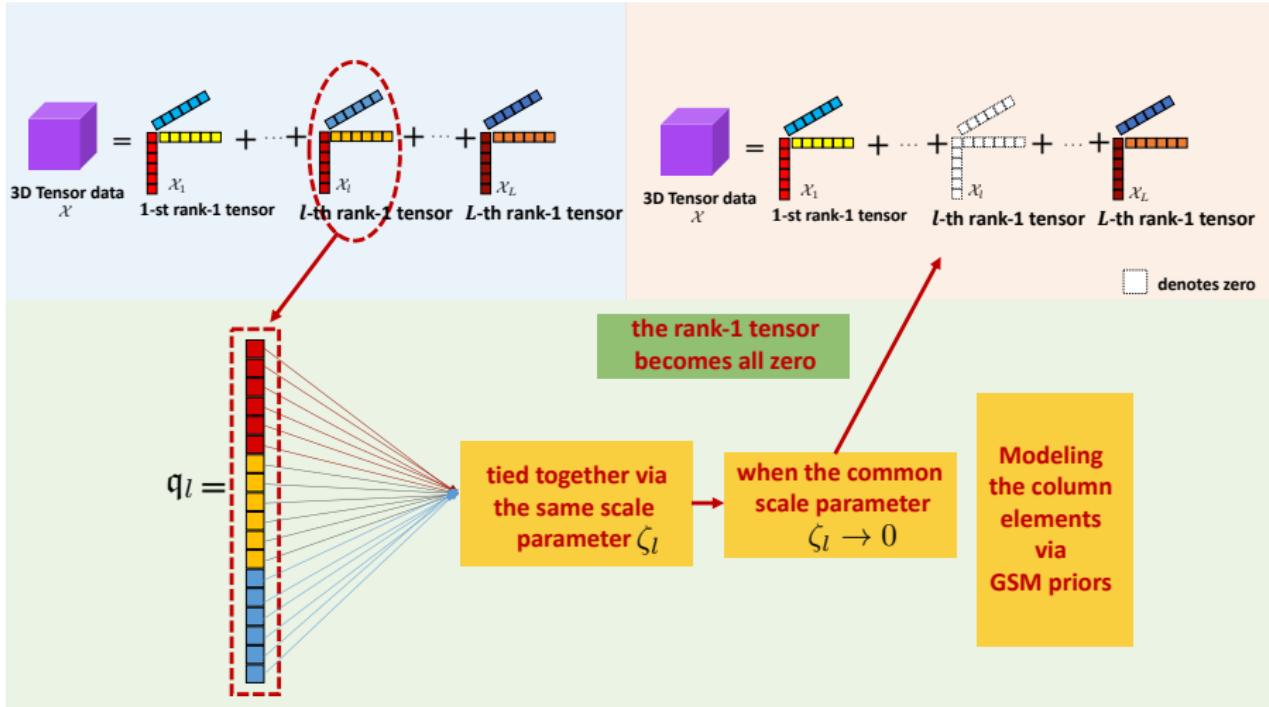
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- To model such sparsity, we adopt the GSM prior:

$$\begin{aligned}
 p(\mathbf{q}_I) &= \int \prod_{i=1}^{\sum_{p=1}^P J_p} \mathcal{N}([\mathbf{q}_I]_i; 0, \zeta_I) p(\zeta_I; \boldsymbol{\eta}_p) d\zeta_I, \\
 &= \int \prod_{p=1}^P \mathcal{N}(\mathbf{a}_I^{(p)}; 0, \zeta_I \mathbf{I}) p(\zeta_I; \boldsymbol{\eta}_p) d\zeta_I.
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 \end{aligned}$$

GSM prior $p(\mathbf{q}_I)$	Mixing distribution $p(\zeta_I)$
Student's <i>t</i>	Inverse Gamma: $p(\zeta_I; \boldsymbol{\eta}_p = [a, b]) = \text{IG}(\zeta_I; a, b)$
Normal-Jefferys	Log-uniform: $p(\zeta_I; \boldsymbol{\eta}_p = [\]) \propto \frac{1}{ \zeta_I }$
Laplacian	Gamma: $p(\zeta_I; \boldsymbol{\eta}_p = [a, b]) = \text{Ga}(\zeta_I; a, b)$
Generalized hyperbolic	Generalized inverse Gaussian: $p(\zeta_I; \boldsymbol{\eta}_p = [a, b, \lambda]) = \text{GIG}(\zeta_I; a, b, \lambda)$
Horseshoe	$\zeta_I = \tau_I v_I, \boldsymbol{\eta}_p = [a, b]$ Half Cauchy: $p(\tau_I) = C^+(0, a)$ $p(v_I) = C^+(0, b)$



Remark 1 (Nonnegative Modeling)

If the factor matrices are further constrained to be **non-negative** for enhanced interpretability in certain applications, simple modification, that is, multiplying a unit-step function $U(a_i^{(p)} \geq 0)$ (which returns one when $a_i^{(p)} \geq 0$ or zero otherwise) to the prior derived in the last slide, can be made to embed both the non-negativeness and the low-rankness¹⁶.

¹⁶ L. Cheng, X. Tong, S. Wang, Y. -C. Wu and H. V. Poor, "Learning Nonnegative Factors From Tensor Data: Probabilistic Modeling and Inference Algorithm," in IEEE Transactions on Signal Processing, vol. 68, pp. 1792-1806, 2020.

Remark 2 (Extensions to Other Tensor Models)

- Similar ideas have been applied to other tensor decomposition models including **Tucker decomposition (TuckerD)** and **tensor train decomposition (TTD)**¹⁷.
- In these works, one first assumes an **over-parameterized model** by setting the model configuration parameters (e.g., multi-linear ranks in TuckerD and TT ranks in TTD) to be large numbers, and then **imposes GSM prior** on the associated model parameters to control the model complexity.

¹⁷ L. Cheng, Z. Chen, and Y.-C. Wu. "Bayesian Tensor Decomposition for Signal Processing and Machine Learning", Springer, 2023.

Inference Algorithms for Bayesian TDs

- Now, we introduce the inference algorithm design for Bayesian tensor decompositions.
- Our focus is on the key ideas for inferring the Bayesian tensor CPD model with the **Gaussian likelihood** and the **GSM prior**.
- For other tensor decomposition formats, the associated inference algorithm follows a similar rationale¹⁷.

¹⁷ L. Cheng, Z. Chen, and Y.-C. Wu. "Bayesian Tensor Decomposition for Signal Processing and Machine Learning", Springer, 2023.

- The goal of inference is to estimate the posterior distributions of factor matrices $\{\mathbf{A}^{(p)} \in \mathbb{R}^{J_p \times L}\}_{p=1}^P$ from possibly incomplete P -D tensor data observations $\mathcal{Y}_\Omega \in \mathbb{R}^{J_1 \times \dots \times J_P}$.
- $\mathcal{Y}_{j_1, \dots, j_P}$ is observed if the P -tuple indices (j_1, \dots, j_P) belongs to Ω .

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- $\mathcal{Y}_{j_1, \dots, j_P}$ is observed if the P -tuple indices (j_1, \dots, j_P) belongs to Ω .
- The forward problem is commonly modeled as a Gaussian likelihood:

$$p(\mathcal{Y}_\Omega | \{\mathbf{A}^{(p)}\}_{p=1}^P; \beta) = \prod_{(j_1, \dots, j_P) \in \Omega} \mathcal{N}(\mathcal{Y}_{j_1, \dots, j_P}; [\mathbf{A}^{(1)}, \dots, \mathbf{A}^{(P)}]_{j_1, \dots, j_P}, \beta^{-1}).$$

- The prior was introduced in previous slides.

Inference Algorithms for Bayesian TDs

- Under the **evidence maximization framework**, the inference problem can be formulated as

$$\mathcal{L}(q(\theta)) \triangleq \int q(\theta) \log \frac{p(\mathcal{D}, \theta)}{q(\theta)} d\theta.$$

- Unknown parameters:

$$\boldsymbol{\theta} \triangleq \{\{\mathbf{A}^{(p)}\}_{p=1}^P, \{\zeta_l\}_{l=1}^L, \beta\}.$$

- The joint pdf:

$$p(\mathcal{D}, \boldsymbol{\theta}) \triangleq p(\mathcal{Y}_\Omega, \{\{\mathbf{A}^{(p)}\}_{p=1}^P, \{\zeta_l\}_{l=1}^L, \beta\}).$$

- To get over the intractable integration difficulty, the ELBO maximization problem is solved by further constraining $q(\theta)$ into a functional family \mathcal{F} , i.e., $q(\theta) \in \mathcal{F}$.
- Among all the functional families, the mean-field family is the most widely used one:

$$q(\theta) = \prod_{p=1}^P q(\mathbf{A}^{(p)}) q(\{\zeta_l\}_{l=1}^L) q(\beta).$$

- Inspect the mean-field family:

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- The factorized structure above inspires the idea of block minimization.
- After fixing the variational pdfs $\{q(\theta_j)\}_{j \neq k}$, the optimal $q(\theta_k)$ was shown to be:

$$q^*(\theta_k) = \frac{\exp \left(\mathbb{E}_{\prod_{j \neq k} q(\theta_j)} [\ln p(\mathcal{D}, \theta)] \right)}{\int \exp \left(\mathbb{E}_{\prod_{j \neq k} q(\theta_j)} [\ln p(\mathcal{D}, \theta)] \right) d\theta_k}.$$

- MF-VI imposes a factorization structure on $q(\theta)$, which implies **statistical independence** of the variables θ_k given observed dataset \mathcal{D} .
- If this is not the case, the mean-field approximation will lead to **mismatch** when approaching the ground-truth posteriors.

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- If this is not the case, the mean-field approximation will lead to **mismatch** when approaching the ground-truth posteriors.
- To achieve more accurate posterior estimation, it is trendy to employ **more advanced** variational approximation techniques, e.g., Stein VI.
- Practical issues:
 - ① informative initial values
 - ② computational complexity
 - ③ low SNR region difficulties
 - ④ etc.

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Section Goals

Finally, we showcase the following practical applications:

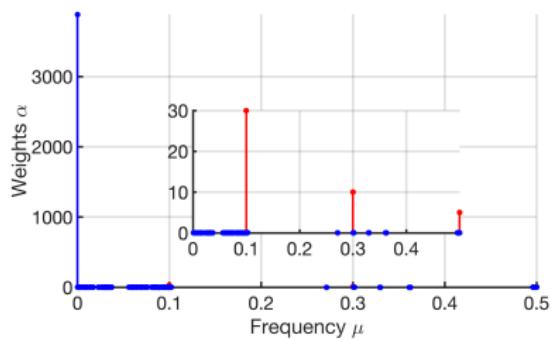
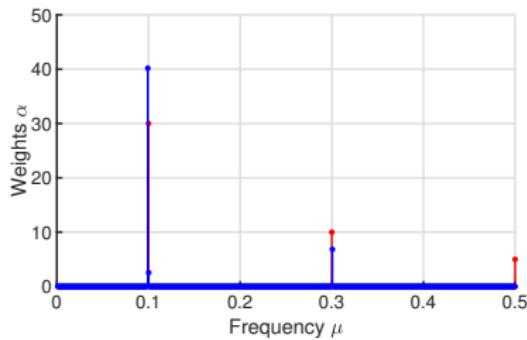
- Time series prediction using Gaussian process (GP) models;
- Adversarial learning using Bayesian deep neural networks (DNNs);
- Social group clustering and image completion using unsupervised tensor decompositions (TDs).

Time Series Prediction via GPs: Classic Datasets

- Consider classic 1D time series datasets with different lengths and evaluate multi-step ahead prediction in terms of MSE.
- Compare the sparsity-promoting GP models (including GSMGP, SSGP, SMGP) with some SOTA time series prediction models.

Name	GSMGP	SSGP	SMGP	LSTM	Informer	ARIMA
	MSE	MSE	MSE	MSE	MSE	MSE
ECG	1.3E - 02	1.6E - 01	1.9E - 02	2.1E - 02	5.4E - 02	1.8E - 01
CO ₂	1.5E + 0	2.0E + 02	1.1E + 0	2.1E + 0	8.4E + 01	4.9E + 0
Electricity	4.7E + 03	8.2E + 03	7.5E + 03	4.7E + 03	8.3E + 03	1.2E + 04
Employment	1.1E + 02	7.7E + 01	0.7E + 02	4.3E + 02	2.0E + 03	3.9E + 02
Hotel	8.9E + 02	1.9E + 04	2.8E + 03	7.8E + 03	2.3E + 04	1.7E + 04
Passenger	1.9E + 02	6.9E + 02	1.6E + 02	1.6E + 02	1.2E + 02	4.5E + 03
Clay	1.9E + 02	5.3E + 02	3.3E + 02	2.7E + 02	1.4E + 02	3.3E + 02
Unemployment	3.6E + 03	2.1E + 04	1.4E + 04	3.5E + 03	3.8E + 03	1.5E + 04

- Synthetic data with three modes.
- Sparse solution identifies the most effective frequency components of the data and, thus, leads to good model interpretability.



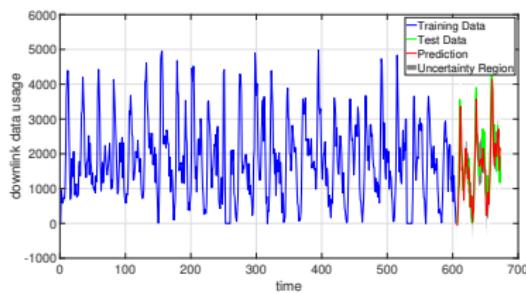
Time Series Prediction via GPs: Real 5G Dataset¹⁸

- Natural uncertainty region of a point prediction for GP models over deterministic models.

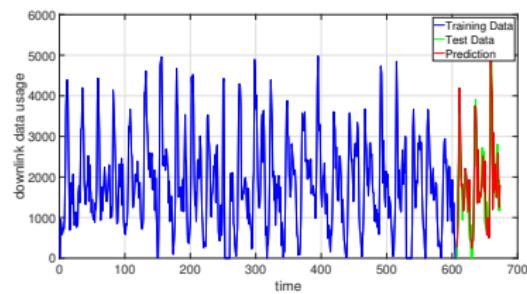
¹⁸ Feng Yin et.al., "Wireless traffic prediction with scalable Gaussian process: Framework, algorithms, and verification", IEEE JSAC, pp.1291-1306,2019.

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GSM based GP



Classic LSTM

- GSMGP with $Q = 500$ fixed grids and $e_{MAPE} = 0.28$; LSTM model with $e_{MAPE} = 1.12$.
- The gray shaded areas represent the uncertainty region of GP model.

¹⁸

Feng Yin et.al., "Wireless traffic prediction with scalable Gaussian process: Framework, algorithms, and verification", IEEE JSAC, pp.1291-1306,2019.

Adversarial Learning via Bayesian DNNs

- Recent studies have revealed that DNNs are highly susceptible to *adversarial examples*, i.e., cleverly crafted examples whose purpose is that of *fooling* a considered model into *misclassification*.

Adversarial Learning via Bayesian DNNs

- Recent studies have revealed that DNNs are highly susceptible to *adversarial examples*, i.e., cleverly crafted examples whose purpose is that of *fooling* a considered model into *misclassification*.
- For example, projected gradient descent (PGD)-based adversarial example construction.
- Under PGD, the obtained perturbed modification to the original example, x , which seems small or even imperceptible to human being, can fool the model to misclassification.

- Drawing upon this vulnerability, **adversarial training** has been recently devoted towards more reliable and robust DNNs.
- Stochastic modeling rationale: Introducing ***stochasticity*** into the considered architecture, e.g., by randomizing the input data and/or the learning model itself.
- Bayesian learning offers a **natural stochastic defense framework** towards more adversarially robust networks.

The so-called **doubly stochastic nature** stems from:

- Sparsity-promoting link-wise non-parametric IBP prior;
 - Stochastic adaptation of the biologically inspired and competition-based LWTA activation.

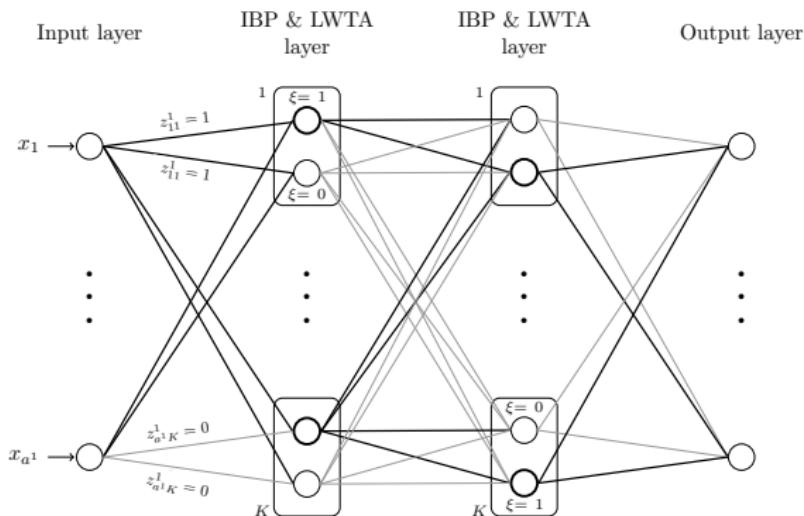


Table: Natural and Robust accuracy under a conventional PGD attack with 20 steps and 0.007 step-size using WideResNet-34 models with different widen factors.

Adversarial Training-PGD					
Widen Factor	Natural Accuracy (%)			Robust Accuracy (%)	
	Baseline	Stochastic	LWTA	Baseline	Stochastic
1	74.04	87.0		49.24	81.87
5	83.95	91.88		54.36	83.4
10	85.41	92.26		55.78	84.3

- **Baseline:** B. Wu *et.al.* “Do wider neural networks really help adversarial robustness?” in Proc. Advances in Neural Information Processing Systems (NeurIPS), 2021.
- Using the same PGD-based Adversarial Training scheme for all models.

Table: Robust Accuracy (%) comparison under the AutoAttack framework.

Method	AutoAttack
HE	53.74
WAR	54.73
Pre-training †	54.92
Data augmentation †	65.88
WAR†	61.84
Stochastic-LWTA/PGD/WideResNet-34-1	74.71
Stochastic-LWTA/PGD/WideResNet-34-5	81.22
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- † denotes models that are trained with additional unlabeled data.
- The AutoAttack performance corresponds to the final robust accuracy after employing all the attacks in AA.

Unsupervised Learning via Bayesian TDs

- We present two unsupervised learning applications:
 - ① Social group clustering: adopts Bayesian tensor CPD;
 - ② Image completion: employs Bayesian tensor TTD.
- Those algorithms **bypass the need of hyper-parameters tuning** and effectively **avoid overfitting**.

Bayesian Tensor CPD for Social Group Clustering

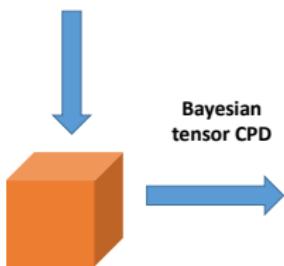
- Dataset: *ENRON E-mail corpus dataset* (a 3-D tensor with the size $184 \times 184 \times 44$ (# of sender, # of receiver, # of day))

Bayesian Tensor CPD for Social Group Clustering

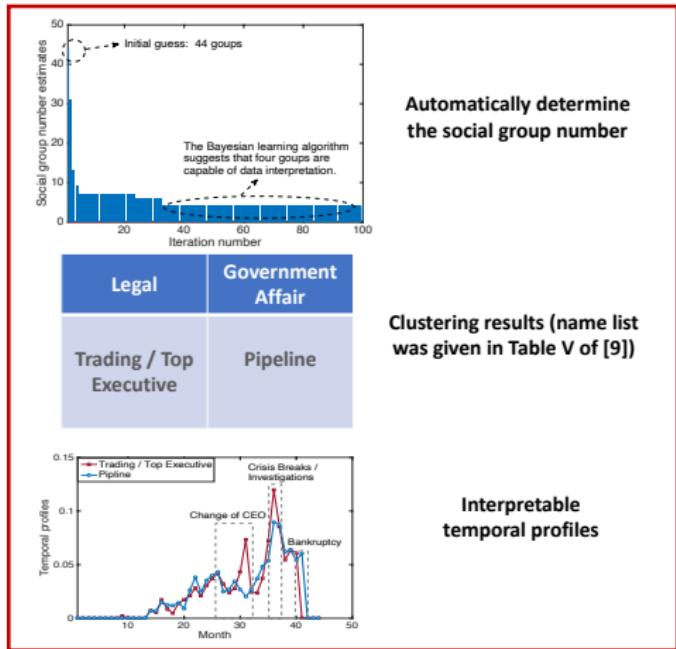
- Dataset: *ENRON E-mail corpus dataset* (a 3-D tensor with the size $184 \times 184 \times 44$ (# of sender, # of receiver, # of day))
- We aim to demonstrate how the Bayesian tensor CPD can be used to simultaneously
 - determine the number of social groups (*automatic tensor rank determination*),
 - cluster people into different groups (*interpretable source separation*),
 - extract interpretable temporal profiles of different social groups (*interpretable source separation*).



Social group clustering



ENRON e-mail corpus



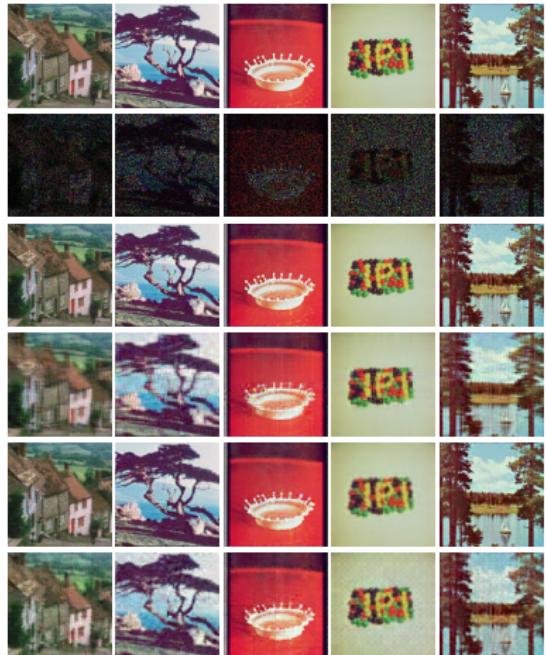
Bayesian Tensor TTD for Image Completion

- Color images are naturally 3-D tensor.
- Fold an image into a higher dimensional tensor (e.g., 9-D tensor), and then apply TTD to recover the missing pixels.

Bayesian Tensor TTD for Image Completion

- Color images are naturally 3-D tensor.
- Fold an image into a higher dimensional tensor (e.g., 9-D tensor), and then apply TTD to recover the missing pixels.
- For a P -D tensor, TTD has $P - 1$ hyper-parameters (called TT ranks).
- Manually tuning different combinations of these hyper-parameters for overfitting avoidance is time-consuming.
- Bayesian TTD, using the ideas introduced before, can automatically learn the most suitable TT-ranks to match the underlying image pattern.

- Experimental results for visual comparison on image completion with 80% missing data.
- Ground-truth images are in the top row.
- The second row includes the images with missing values.
- The third to the bottom rows include results from Bayesian TTD, TTC-TV, TMAC-TT, and STTO.



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Conclusion

- Presented a gentle overview of state-of-the-art sparsity-promoting priors for both Bayesian parametric and nonparametric models.
- Constrained our focus to modern GP models, Bayesian DNNs, and TDs.
- Introduced advanced prior design strategies and inference algorithms.
- Demonstrated a wide spectrum of signal processing and machine learning applications.

The reported results indicated that:

- ① Sparsity-promoting priors are adaptive to varying data and enable automatic model structure selection;
- ② Sparsity-promoting priors lead to natural and reasonable uncertainty quantification;
- ③ Sparse solution can better reveal the underlying characteristics of a target system/signal with the most effective components.

Future Directions

Potential challenges include but not limited to:

- Quality of the posterior/predictive distribution, compared with that provided by conformal prediction.
- Issues with misspecification of the learning model and noise statistics.
- Emerging sparsity-promoting mechanisms inspired from neuroscience.
- More emerging applications in complex systems, such as 6G, ISAC, autonomous driving system, ocean sensing, etc.
- Sparsity-awareness in emerging learning paradigms and large language models (LLMs).

Thanks for your attention!

