Short Bio

2009-2015: Bachelor and Master of statistics, minor in computer science. LMU Munich.
2014-2018: Dr. rer. nat. in computer science. LMU Munich, supervised by Prof. Dr. Volker Tresp.

2018-2022: Research Scientist at Siemens AG, Munich.
2022- : Senior Key Expert for robust AI at Siemens AG, Munich.
2019- : Co-lecturer “Deep Learning and AI” at LMU Munich.

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Tensorization and uncertainty quantification in Deep Learning

Dr. Yinchong Yang, Siemens AG

Invited Talk at Cyprus Institute, 2023-05-23

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Tensorization of neural networks in Deep Learning

“Representing large weight matrices in NN with product of small tensors…”

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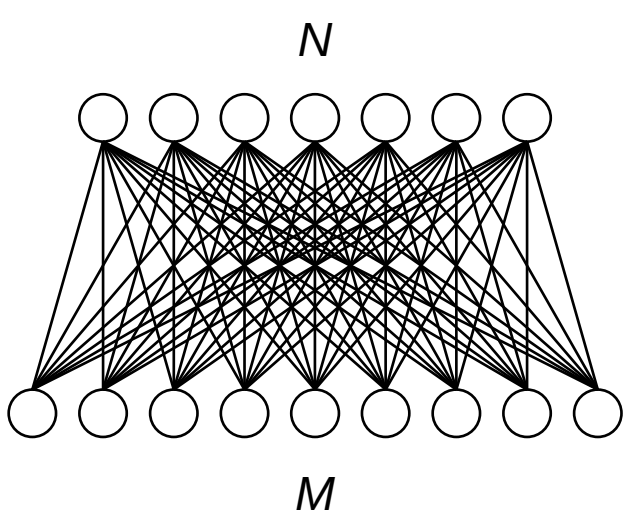
A motivating example



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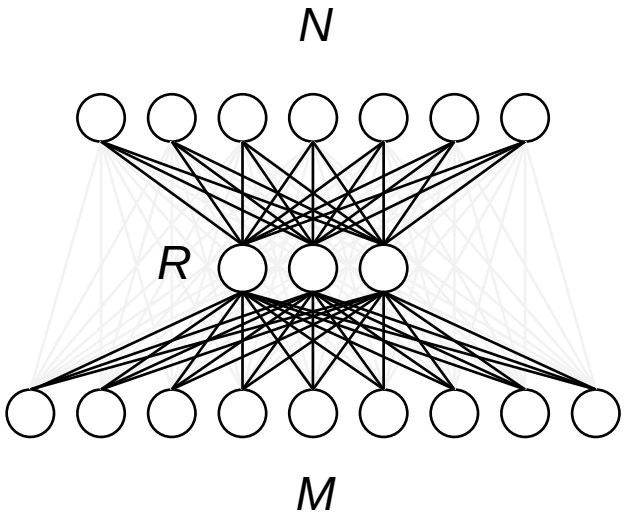

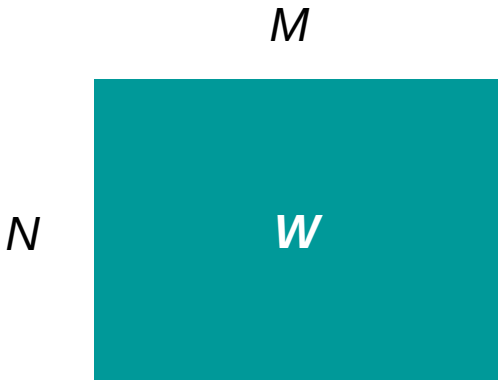

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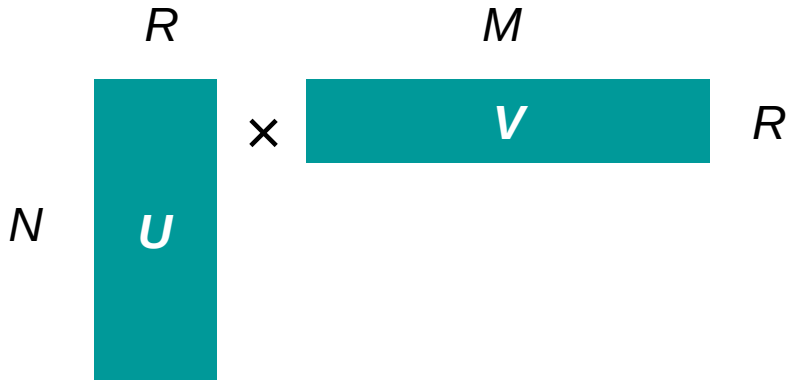

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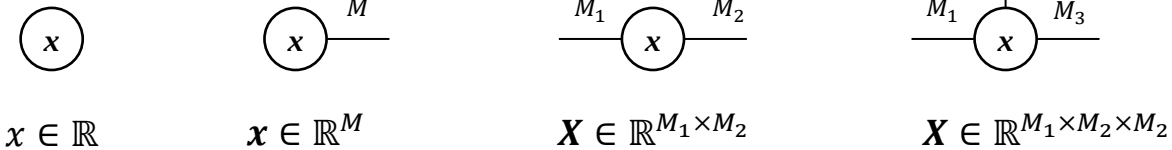
Preliminary: Tensor Graph and Einstein Summation Notation

In the syntax of tensor graph notation:

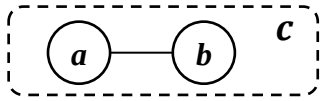
- Node = tensor
- Edge = “mode” / dimensionality

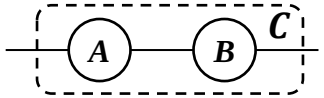


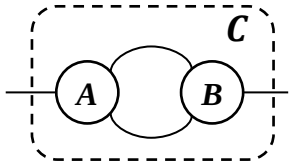
$x \in \mathbb{R}$ $\quad \boldsymbol{x} \in \mathbb{R}^{M}$ $\quad \boldsymbol{X} \in \mathbb{R}^{M_1 \times M_2}$ $\quad \boldsymbol{X} \in \mathbb{R}^{M_1 \times M_2 \times M_2}$

- Connection = tensor contraction
  - Combining multiple tensors to form a new one.
  - A graph representation of Einstein’s summation.

Tensor graph notation	Matrix notation	Einstein summation notation	pytorch

	$c = \langle \boldsymbol{a}, \boldsymbol{b} \rangle$	$c = a(n)b(n)$	`a = torch.randn(5)`
			`b = torch.randn(5)`
			`torch.einsum('n,n->', a, b)`
			`# torch.inner(a, b)`

	$\boldsymbol{C} = \boldsymbol{AB}$	$\boldsymbol{C}(m,k) = \boldsymbol{A}(m,n)\boldsymbol{B}(n,k)$	`A = torch.randn(3, 5)`
			`B = torch.randn(5, 4)`
			`torch.einsum('mn,nk->mk', A, B)`
			`# torch.matmul(A, B)`

	?	$\boldsymbol{C}(n,r) = \boldsymbol{A}(m,n,k)\boldsymbol{B}(m,k,r)$	`A = torch.randn(5, 10, 7)`
			`B = torch.randn(5, 7, 2)`
			`torch.einsum('mnk,mkr->nr', A, B)`

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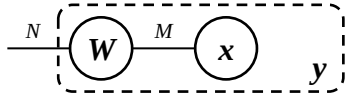
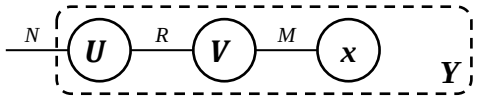
Tensorized neural networks

- A fully connected layer (omitting the bias) $\boldsymbol{y} = \boldsymbol{W}\boldsymbol{x}$ can be formulated as contraction:
  - $\boldsymbol{y}(n) = \boldsymbol{W}(n,m)\boldsymbol{x}(m)$, with $\boldsymbol{W} \in \mathbb{R}^{N\times M}, \boldsymbol{x} \in \mathbb{R}^{M}$.
  - Size: $N \times M$.

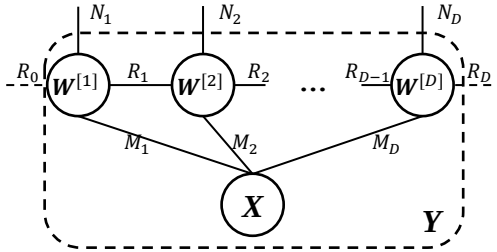


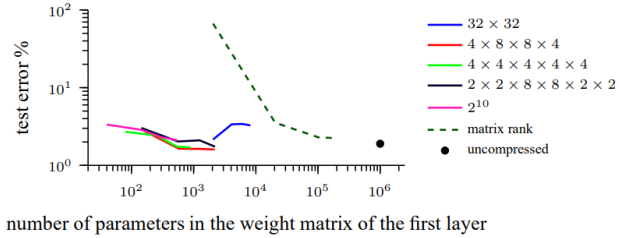
- A bottleneck FC layer as:
  - $\boldsymbol{y}(n) = \boldsymbol{V}(n,r)\boldsymbol{U}(r,m)\boldsymbol{x}(m)$ with $\boldsymbol{V} \in \mathbb{R}^{N\times R}, \boldsymbol{U} \in \mathbb{R}^{R\times M}, \boldsymbol{x} \in \mathbb{R}^{M}$.
  - Size: $R \times (M + N)$.



- A tensor-train layer [Novikov et al. 2015] closely related to Matrix Product State.
  - $\boldsymbol{y}(n_1, n_2, \ldots, n_D) =$
    $\boldsymbol{W}^{[D]}(n_D, r_{D-1}, r_D, m_D) \ldots \boldsymbol{W}^{[2]}(n_2, r_1, r_2, m_2)\, \boldsymbol{W}^{[1]}(n_1, r_0, r_1, m_1)\, \boldsymbol{x}(m_1, m_2, \ldots, m_D),$
  - Size: $\sum_{d=1}^{D} M_d N_d R_{d-1} R_d$ instead of $\mathrm{M} \times N = \prod_{d=1}^{D} M_d N_d$

$$M = M_1 \times M_2 \times \ldots \times M_D$$
$$N = N_1 \times N_2 \times \ldots \times N_D$$





Novikov, Alexander, et al. "Tensorizing neural networks." *NeurIPS* 2015.

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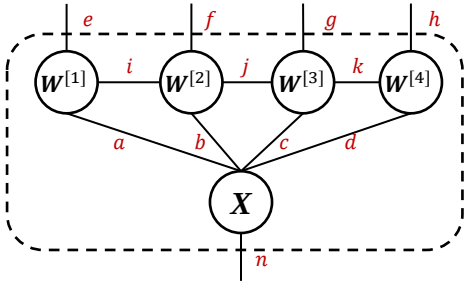
Tensorized neural networks

- Implementation in pytorch:
  - Step 1: decide the decomposition of input and output modes, as well as the rank.
    - Example: 4096 → 16 can be decomposed into $(8 \times 8 \times 8 \times 8) \rightarrow (2 \times 2 \times 2 \times 2)$ with rank 2
  - Step 2: draw a tensor train layer and name the edges.
    - Example:




```
opt = torch.optim.Adam([W1, W2, W3, W4], lr=5e-2)
loss = torch.nn.MSELoss()

for i in range(10000):
    y_hat = torch.einsum('aei, bfij, cgjk, dhk, nabcd -> nefgh', W1, W2, W3, W4, X)
    error = loss(y_hat.reshape(n_samples, -1), y.reshape(n_samples, -1))
    error.backward()
    opt.step()
    opt.zero_grad()
```

  - Step 3: implement an torch.einsum operation with given names in step 2.
  - Step 4: implement the backward pass.

Tensorized neural networks

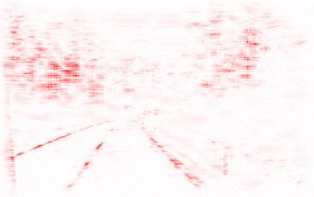
	Accuracy	# Parameters	Runtime
TT-MLP	0.427 ± 0.045	7,680	902s
GRU	0.488 ± 0.033	44,236,800	7,056s
LSTM	0.492 ± 0.026	58,982,400	8,892s
TT-GRU	**0.813 ± 0.011**	3,232	1,872s
TT-LSTM	0.796 ± 0.035	3,360	2,160s

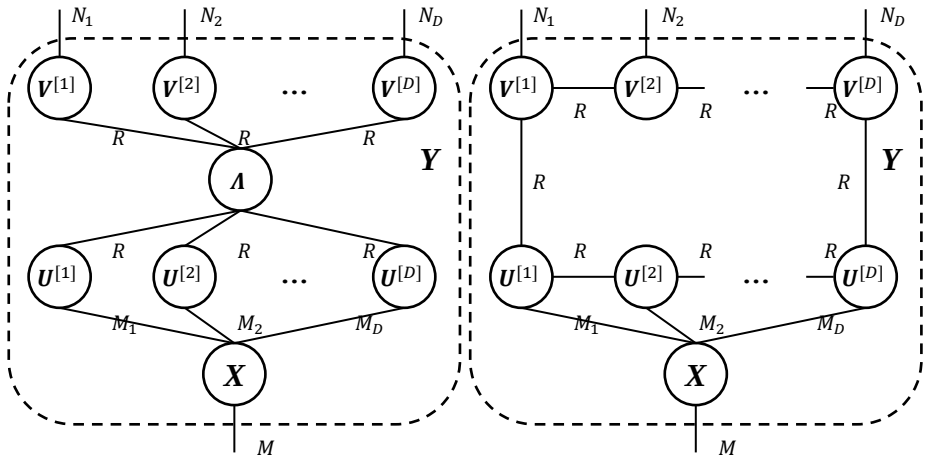
Original: (Liu et al., 2009)	0.712
(Liu et al., 2013)	0.761
(Hasan & Roy-Chowdhury, 2014)	0.690
(Sharma et al., 2015)	**0.850**
Our best model (TT-GRU)	0.813

- Line of research: new architectures based on tensorized neural network:
  - Tensorized CNN [Garipov et al. 2016],
  - Tensorized RNN [Yang et al. 2017, Tjandra et al. 2017],

- Line of research: new applications:
  - Time series data [Yu et al. 2017]
  - Video data – e.g. autonomous driving (contribution by Max Pittner) with LRP.
  - Sparse tabular data [Yang et al. 2017]

- Line of research: other decompositions
  - CP and Tucker [Pan et al. 2023] (left)
  - Tensor-Ring [Wang et al. 2018] (right)





Garipov, Timur, et al. "Ultimate tensorization: compressing convolutional and fc layers alike." *NeurIPS* (2016) *Workshop*.
Tjandra, Andros, Sakriani Sakti, and Satoshi Nakamura. "Compressing recurrent neural network with tensor train." *2017 International Joint Conference on Neural Networks (IJCNN)*. IEEE, 2017.
Yu, Rose, et al. "Long-term forecasting using tensor-train rnns." *Arxiv* (2017).
Yang, et al. "Modeling progression free survival in breast cancer with tensorized recurrent neural networks and accelerated failure time models." MLHC, PMLR, 2017.
Pan et al. https://tednet.readthedocs.io/en/latest/ visited on 2023-05-18
Wang, Wenqi, et al. "Wide compression: Tensor ring nets." *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*. 2018.

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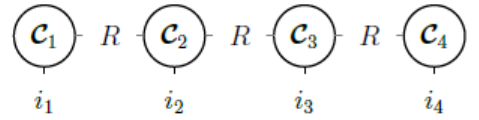
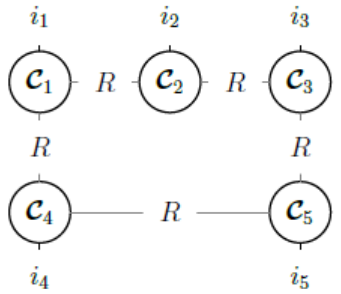
Tensorized neural networks

$$\boldsymbol{A}_{TT} = \begin{pmatrix} 0 & R & 0 & 0 \\ R & 0 & R & 0 \\ 0 & R & 0 & R \\ 0 & 0 & R & 0 \end{pmatrix} \equiv$$

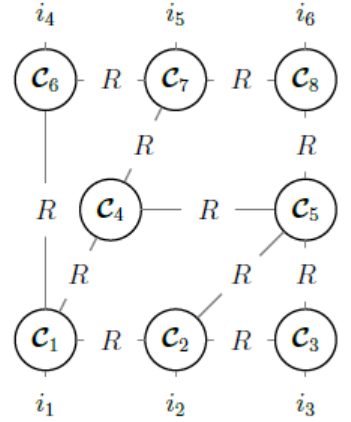


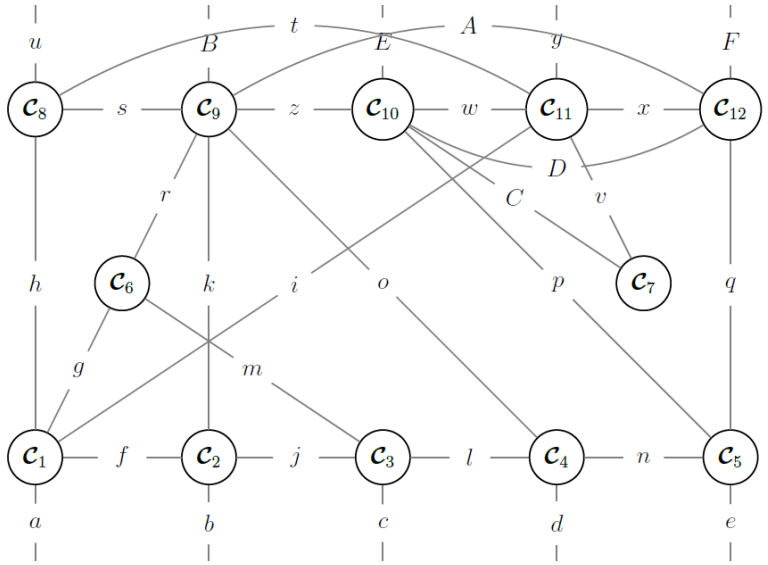
- Flexible topology [Li and Sun 2020, Master thesis Arber Qoku]
  - Representing the core tensor topology with adjacency matrix (vectorized lower-/upper triangle).
  - Optimize the topology of core tensors as a hyper-parameter via evolution strategy and Bayesian optimization:

$$\boldsymbol{A}_{TR} = \begin{pmatrix} 0 & R & 0 & R & 0 \\ R & 0 & R & 0 & 0 \\ 0 & R & 0 & 0 & R \\ R & 0 & 0 & 0 & R \\ 0 & 0 & R & R & 0 \end{pmatrix} \equiv$$



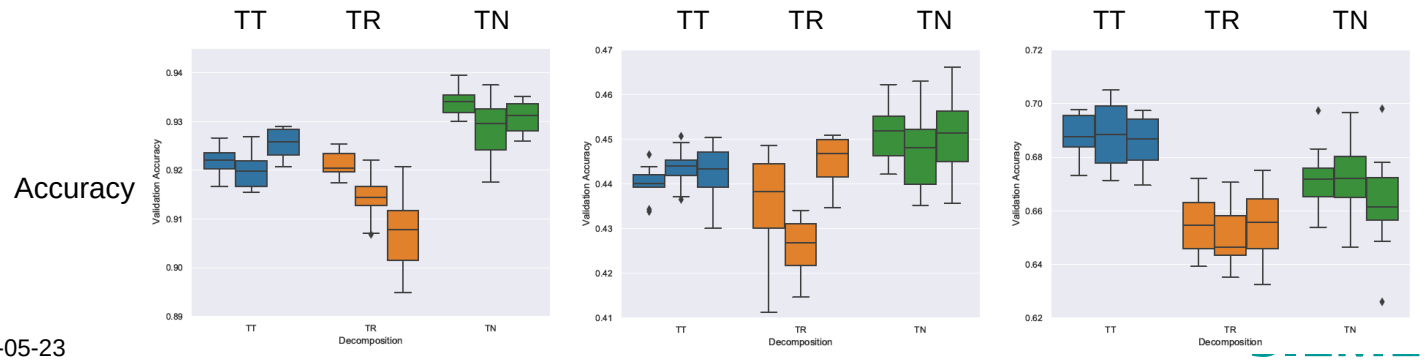
$$\boldsymbol{A}_{TN} = \begin{pmatrix} 0 & R & 0 & R & 0 & R & 0 & 0 \\ R & 0 & R & 0 & R & 0 & 0 & 0 \\ 0 & R & 0 & 0 & R & 0 & 0 & 0 \\ R & 0 & 0 & 0 & R & 0 & R & 0 \\ 0 & R & R & R & 0 & 0 & 0 & R \\ R & 0 & 0 & 0 & 0 & 0 & R & 0 \\ 0 & 0 & 0 & R & 0 & R & 0 & R \\ 0 & 0 & 0 & 0 & R & 0 & R & 0 \end{pmatrix} \equiv$$





Random Search
Bayesian optimization
Evolution strategy

MNIST CIFAR10 Paul15



Li, Chao, and Zhun Sun. Evolutionary topology search for tensor network decomposition. *ICML*, 2020.

Uncertainty quantification with GP in Deep Learning

“Combining the predictive distribution of GP with representation learning by NN.”

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Gaussian Processes Recap

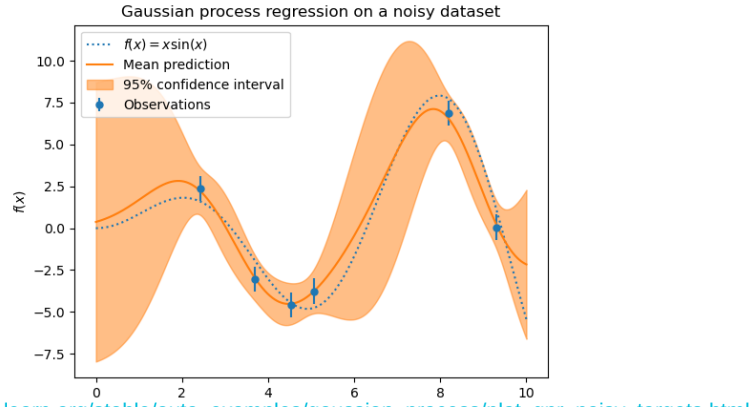
- Standard Gaussian Process regression:
  - $p(y_*|\boldsymbol{x}_*, D) = \int p(y_*|\boldsymbol{x}_*, \boldsymbol{\theta}) p(\boldsymbol{\theta}|D) d\boldsymbol{\theta}$

$$= N(\frac{1}{\sigma^2}\boldsymbol{k}_*^T(\boldsymbol{K} + \sigma^2\boldsymbol{I})^{-1}\boldsymbol{y}, k_{**} - \boldsymbol{k}_*^T(\boldsymbol{K} + \sigma^2\boldsymbol{I})^{-1}\boldsymbol{k}_* + \sigma^2)$$

with

$$\boldsymbol{k}_* = (k(\boldsymbol{x}_*, \boldsymbol{x}_i))_{i=1}^n \epsilon \mathbb{R}^n \text{ and } \boldsymbol{K} = \left(k(\boldsymbol{x}_i, \boldsymbol{x}_j)\right)_{i=1,j=1}^{n,n} \epsilon \mathbb{R}^{n \times n}$$

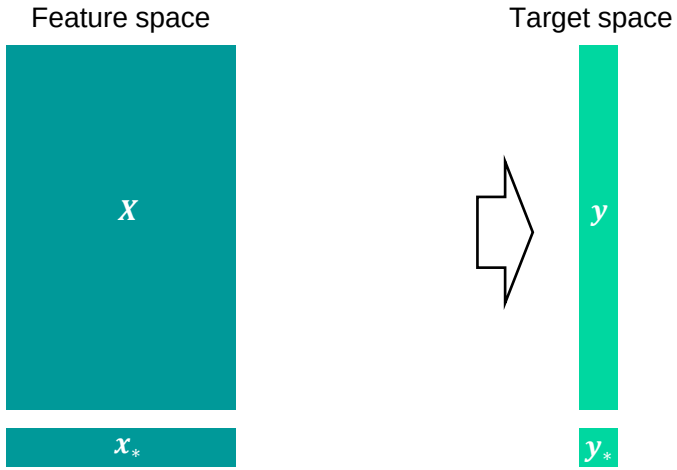
being the kernel function that measures the similarity between data points.



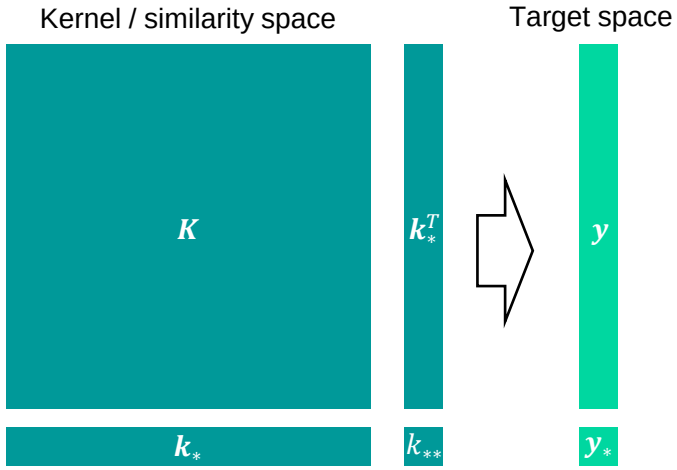
https://scikit-learn.org/stable/auto_examples/gaussian_process/plot_gpr_noisy_targets.html

- The computational complexity is $\boldsymbol{O}(n^3)$ due to the matrix inverse.

Parametric models:



Non-Parametric models:



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Scalable Gaussian Processes

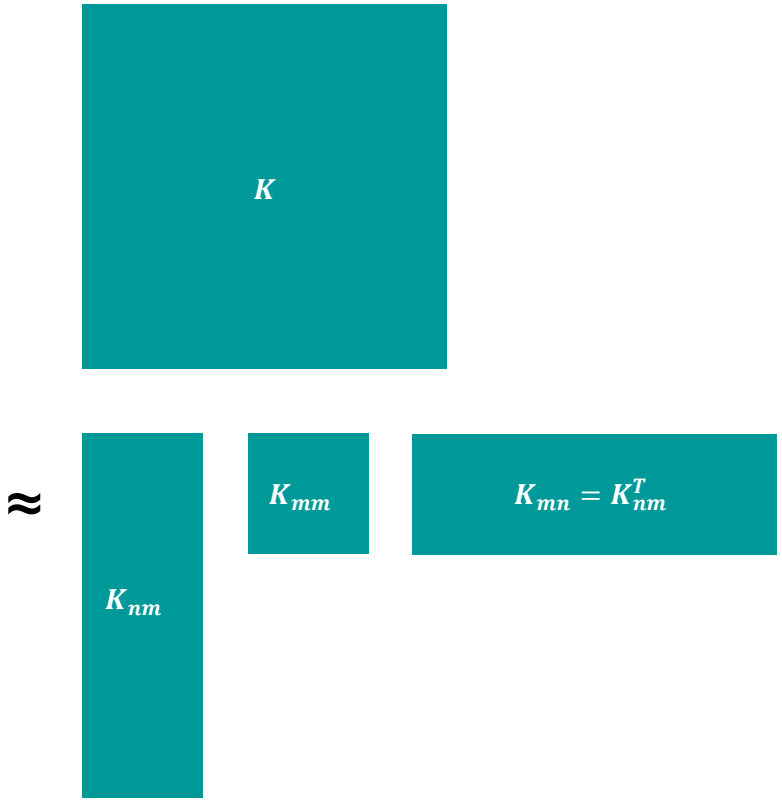
- Various approaches have been proposed to approximate the full covariance matrix. But the idea remains the same: representing the whole training set with a few "*inducing points*":

$$\boldsymbol{K} \approx \boldsymbol{Q} = \boldsymbol{K}_{nm}\boldsymbol{K}_{mm}^{-1}\boldsymbol{K}_{mn}$$

  so that it can be inverted using the Woodbury formula [Williams & Seeger 2000]. That is,

$$k(\boldsymbol{x}_i, \boldsymbol{x}_j) \approx \boldsymbol{k}(\boldsymbol{x}_i, \boldsymbol{Z})^T \boldsymbol{K}_{mm}^{-1} \boldsymbol{k}(\boldsymbol{x}_j, \boldsymbol{Z})$$

- The set of inducing points $\boldsymbol{Z}$ could also be learned as parameter:
  - FITC [Snelson et al. 2000]
  - VFE [Titias 2009]
  - SVGP [Hensman et al. 2013]
  - PPGP [Jankowiak et al. 2020]



Williams and Seeger. Using the Nyström method to speed up kernel machines. *NeurIPs* 2000.
Snelson et al. Sparse Gaussian processes using pseudo-inputs. *NeurIPs*. 2006.
Titsias. Variational learning of inducing variables in sparse Gaussian processes. *AISTATS* 2009.
Hensman et al. Gaussian Processes for Big Data. *UAI.* 2013.
Jankowiak et al. Parametric gaussian process regressors. *ICML*, 2020.

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Scalable Gaussian Processes for collaborative filtering

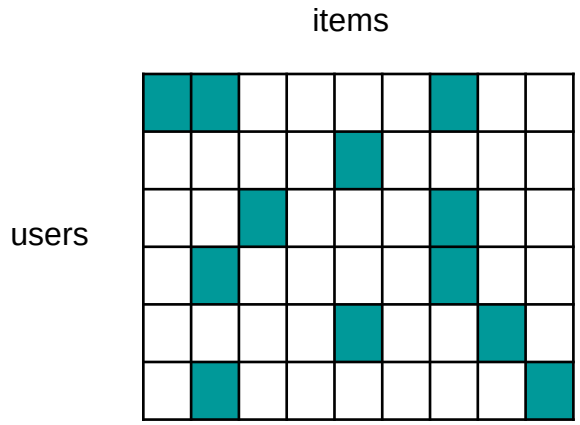
- Collaborative filtering: modeling user-item interaction, applied in recommender systems.
- Classical approaches include matrix decomposition such as SVD and NMF, more advanced methods such as multiway NN [Nickel et al. 2015].

$$y_{i,j} = f(\boldsymbol{a}_i, \boldsymbol{b}_j)$$

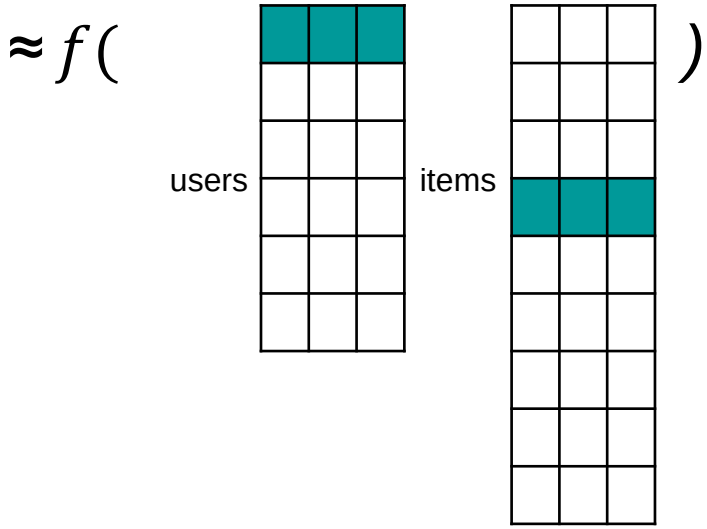
  - with

$$\boldsymbol{Y} \in \mathbb{R}^{I \times J}, \boldsymbol{A} \in \mathbb{R}^{I \times r}, \boldsymbol{B} \in \mathbb{R}^{I \times r}$$

- The expressiveness of the model depends on the choice of function f.



- GP-LVM is one of the very few methods are capable of expressing predictive uncertainty, but doesn't scale well to large and sparse user-item matrices.



Nickel, Maximilian, et al. A review of relational machine learning for knowledge graphs. *Proceedings of the IEEE* 104.1 (2015): 11-33.

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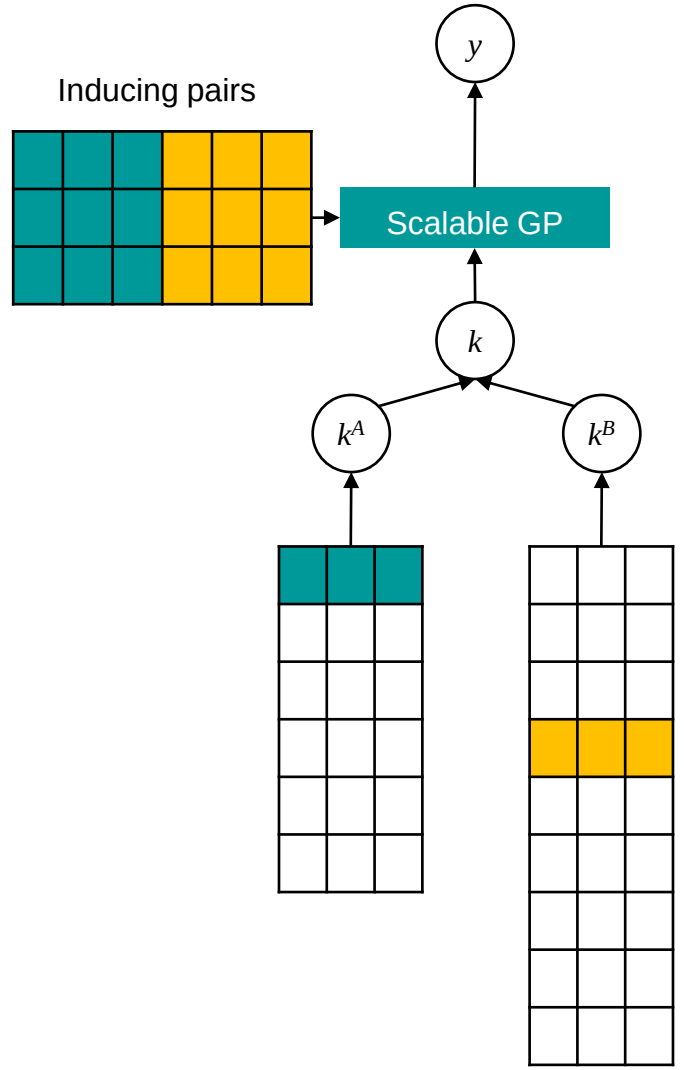
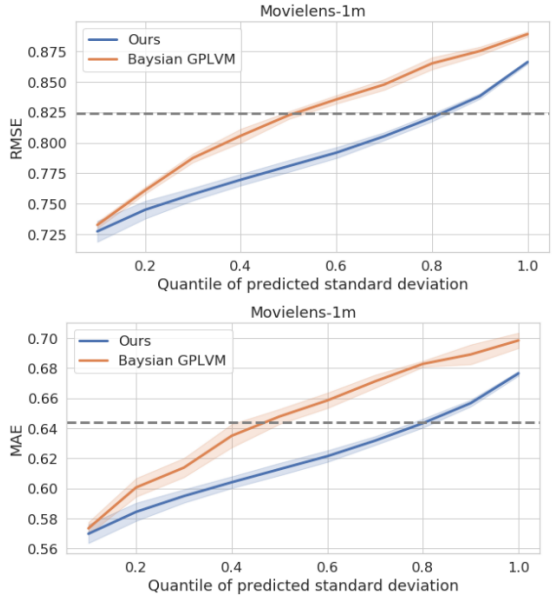
Scalable Gaussian Processes for collaborative filtering

- Our proposal: let f be a Gaussian Process regression and learn the embeddings jointly.

- Challenges and solutions:
  - Kernels → Define two kernels for $\boldsymbol{A}$ and $\boldsymbol{B}$ respectively.
  - Scalability (up to 10 million) → SOTA scalable GP.
  - Inducing points → "*inducing pairs*", initialized via kernel PCA
  - Evaluation → Quantile-Performance-Plot



	RMSE	MAE
CF-NADE [Zheng et al., 2016]	0.829	-
GPLVM [Lawrence and Urtasun, 2009]	0.880	**0.644**
Sparse FC [Muller et al., 2018]	**0.824**	-
GC [Berg et al., 2017]	0.832	-
CWOCF [Lu et al., 2013]	0.958	0.761
LLORMA [Lee et al., 2013]	0.865	-
Biased MF	0.863	0.678
SVD++	0.893	0.705
Bayesian GPLVM at $q = 100\%$	0.889	0.698
MW-GP at $q = 100\%$	0.866	0.676
MW-GP at $q = 90\%$	0.838	0.657
MW-GP at $q = 80\%$	0.821	0.643



Yang and Buettner. Multi-output gaussian processes for uncertainty-aware recommender systems. *UAI*. 2021.

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Scalable Gaussian Processes for Deep Neural Networks

- CNN + Scalable GP:

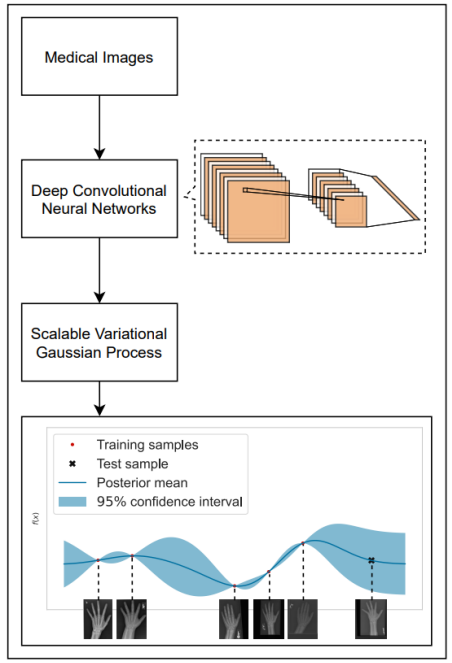


TABLE I
BONE AGE PREDICTION WITH DENSENET121

Output Layer	Transfer Learning	RMSE (No pre-training)	RMSE (DML)	RMSE (CAE)
Linear*	Yes	12.118 ± 0.277	11.667 ± 0.231	14.076 ± 0.281
SVGP†	Yes	11.697 ± 0.102	$\mathbf{11.440 \pm 0.132}$	$\mathbf{13.536 \pm 0.279}$
PPGP†	Yes	$\mathbf{11.679 \pm 0.061}$	11.529 ± 0.089	13.694 ± 0.274
Linear*	No	19.934 ± 0.246	$\mathbf{15.805 \pm 0.157}$	15.340 ± 0.390
SVGP†	No	$\mathbf{17.723 \pm 0.298}$	15.832 ± 0.284	$\mathbf{15.323 \pm 0.411}$
PPGP†	No	18.341 ± 0.234	16.084 ± 0.336	15.752 ± 0.352

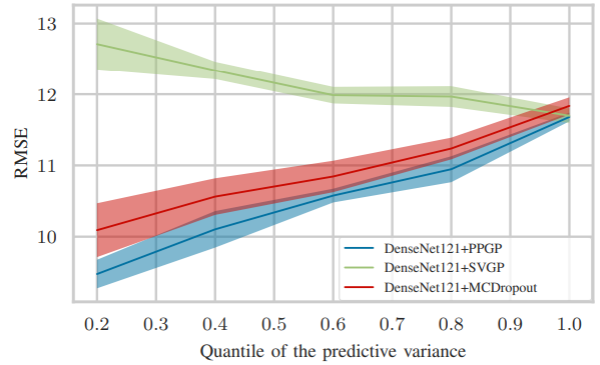
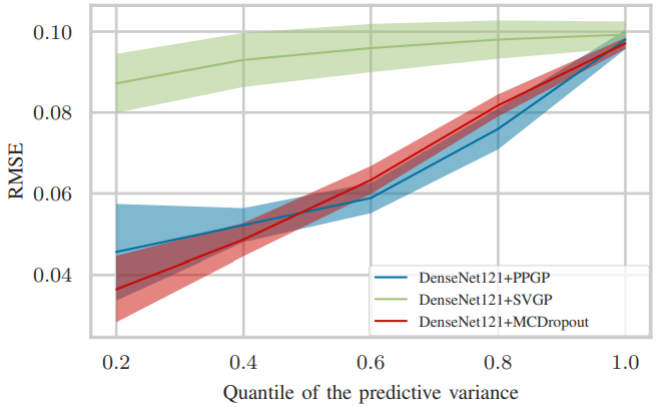


TABLE II
LESION LOCALIZATION WITH DENSENET121

Output Layer	Transfer Learning	RMSE (No pre-training)	RMSE (Metric)	RMSE (CAE)
Linear*	Yes	0.102 ± 0.002	0.101 ± 0.002	0.102 ± 0.003
SVGP†	Yes	0.099 ± 0.003	0.101 ± 0.003	0.104 ± 0.004
PPGP†	Yes	$\mathbf{0.098 \pm 0.002}$	$\mathbf{0.098 \pm 0.002}$	$\mathbf{0.099 \pm 0.002}$
Linear*	No	0.116 ± 0.001	0.114 ± 0.003	0.114 ± 0.002
SVGP†	No	0.118 ± 0.002	0.114 ± 0.003	0.112 ± 0.003
PPGP†	No	$\mathbf{0.115 \pm 0.002}$	$\mathbf{0.111 \pm 0.005}$	$\mathbf{0.110 \pm 0.002}$



- Tasks: Bone-age prediction, lesion localization.
- Challenge: inducing points initialization.
- Solution: pre-training with auto-encoders.

Wu, et al. Quantifying predictive uncertainty in medical image analysis with deep kernel learning. *2021 IEEE ICHI*. 2021.

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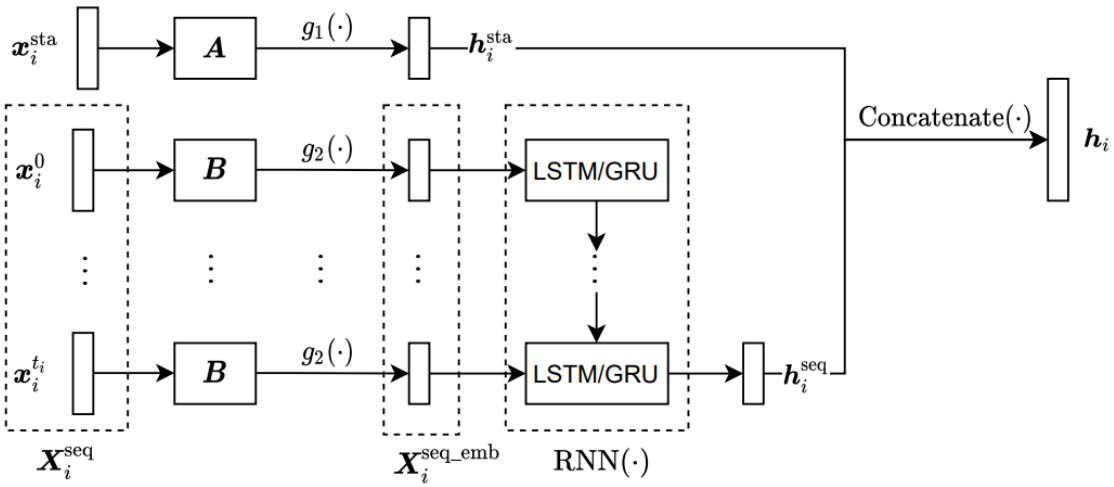
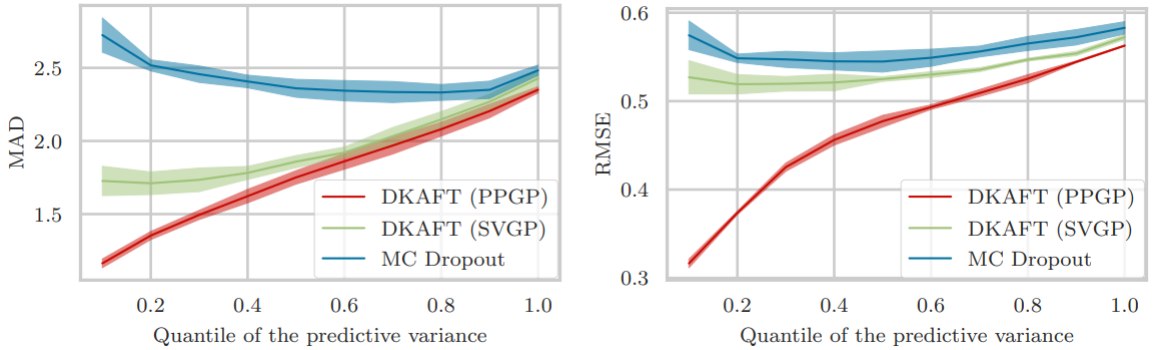
Scalable Gaussian Processes for Deep Neural Networks

- RNN + Scalable GP



Method	Pre-training	Progression-Free Survival MAD	Progression-Free Survival RMSE	Length-of-Stay MAD	Length-of-Stay RMSE
Cox Regression	–*	200.800 ± 16.984	1.609 ± 0.054	2.727 ± 0.007	0.638 ± 0.0002
AFT Regression	–*	206.065 ± 8.988	1.685 ± 0.080	2.742 ± 0.014	0.630 ± 0.0001
RNN+AFT	None	150.918 ± 3.009	1.273 ± 0.019	2.476 ± 0.040	0.575 ± 0.003
DKAFT (ExactGP)	None	144.622 ± 8.689	1.225 ± 0.022	–†	–†
DKAFT (SVGP)	None	154.237 ± 13.490	1.211 ± 0.020	2.428 ± 0.056	0.572 ± 0.003
DKAFT (PPGP)	None	147.108 ± 6.284	1.220 ± 0.019	2.351 ± 0.021	0.563 ± 0.001
RNN+AFT	DML	138.155 ± 7.496	1.267 ± 0.007	2.452 ± 0.057	0.568 ± 0.001
DKAFT (ExactGP)	DML	$\mathbf{134.422 \pm 7.255}$	1.202 ± 0.012	–†	–†
DKAFT (SVGP)	DML	151.852 ± 11.305	1.221 ± 0.007	2.438 ± 0.079	0.567 ± 0.005
DKAFT (PPGP)	DML	146.616 ± 17.109	$\mathbf{1.195 \pm 0.008}$	$\mathbf{2.346 \pm 0.042}$	$\mathbf{0.557 \pm 0.002}$



- Tasks: Progression-free survival, length of stay [Sources]
- Challenge: inducing points initialization
- Solution: pre-training, esp. the deep metric learning:

$$\mathcal{J}_{\text{triplet}} = \sum_{i=1}^{n} \left[\mathrm{d}(\boldsymbol{h}_i^{\mathrm{A}}, \boldsymbol{h}_i^{\mathrm{P}}) - \mathrm{d}(\boldsymbol{h}_i^{\mathrm{A}}, \boldsymbol{h}_i^{\mathrm{N}}) + \alpha \right]_+,$$

Wu, et al. Uncertainty-Aware Time-to-Event Prediction using Deep Kernel Accelerated Failure Time Models. *MLHC (JMLR)*. 2021.

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