Supervised machine learning with tensor-based kernel machines

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Setting the stage...

Parametric supervised learning problem:

Given a set of measurements $\{(\boldsymbol{x}_n, y_n)\}_{n=1}^N$ and a parameterization $\boldsymbol{w}$ of $\hat{y}_n(\cdot)$ in

$$y_n = \hat{y}_n(\boldsymbol{x}_n | \boldsymbol{w}) + e_n,$$

determine $\boldsymbol{w}$.

Kernel machines

$$\hat{y}_n(\boldsymbol{x}_n|\boldsymbol{w}) = \varphi(\boldsymbol{x}_n)^T\ \boldsymbol{w}$$

$\varphi(\cdot)$: collection of basis functions

LTI systems

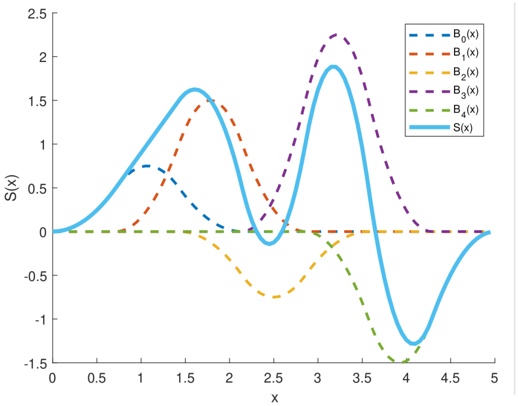
$$\text{OE:} \quad \hat{y}_n = \begin{pmatrix} u_n & \cdots & \hat{y}_{n-1} & \cdots \end{pmatrix} \boldsymbol{w}$$

$$\text{ARMAX/ Box Jenkins:} \quad \hat{y}_n = \begin{pmatrix} u_n & \cdots & y_{n-1} & \cdots & \hat{y}_{n-1} & \cdots \end{pmatrix} \boldsymbol{w}$$

$\Rightarrow$ Learn $\boldsymbol{w}$ from data = solving multivariate polynomial system

Pick your favorite basis function

$$\hat{y}(x) = w_0\ B_0(x) + w_1\ B_1(x) + w_2\ B_2(x) + w_3\ B_3(x) + \cdots$$



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A simple univariate example

$$\hat{y}(x) = w_0 + w_1\, x + w_2\, x^2$$

$$= \underbrace{\begin{pmatrix} 1 & x & x^2 \end{pmatrix}}_{\varphi(x)^T} \underbrace{\begin{pmatrix} w_0 \\ w_1 \\ w_2 \end{pmatrix}}_{\boldsymbol{w}}$$

Another simple univariate example

Ground truth:

$$y = f(x) + e = 3.2\,x^2 - 9.6\,\cos\left(5.1\,x^3 - e^{-3\,x}\right) + e$$

Assume $x \in [-1, 1]$. How many basis functions I do we need?

$$f(x) = 3.2\,x^2 - 9.6\,\cos\left(5.1\,x^3 - e^{-3\,x}\right) \approx \sum_{i=1}^{I} \varphi_i(x)\,w_i$$

The total number of basis functions I we need depends on $\varphi_i(x)$ and $f(x)$.

Multivariate basis functions as products of univariate basis functions

$$\underbrace{\varphi(\boldsymbol{x})}_{I^D} = \underbrace{\varphi(x_1)}_{I} \otimes \underbrace{\varphi(x_2)}_{I} \otimes \cdots \otimes \underbrace{\varphi(x_D)}_{I}$$

Bivariate monomial basis functions from a Kronecker product

$$\varphi(\boldsymbol{x}) = \varphi(x_1) \otimes \varphi(x_2)$$

$$\begin{pmatrix} 1 \\ x_1 \\ x_1^2 \\ x_2 \\ x_1 x_2 \\ x_1^2 x_2 \\ x_2^2 \\ x_1 x_2^2 \\ x_1^2 x_2^2 \end{pmatrix} = \begin{pmatrix} 1 \\ x_1 \\ x_1^2 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ x_2 \\ x_2^2 \end{pmatrix}$$

Learning problem

$$\boldsymbol{y} = \boldsymbol{\Phi}\, \boldsymbol{w} + \boldsymbol{e}$$

$$\min_{\boldsymbol{w}} L(\boldsymbol{y}, \boldsymbol{\Phi}, \boldsymbol{w})$$

Possible loss functions $L(\boldsymbol{y}, \boldsymbol{\Phi}, \boldsymbol{w})$:

- logistic (logistic regression)
- hinge (support vector machines / classification)
- Vapnik ϵ-insensitive (support vector machines / regression)
- squared (least-squares support vector machines, Gaussian Processes)

Squared loss

$$\min_{\boldsymbol{w}} ||\boldsymbol{y} - \boldsymbol{\Phi}\ \boldsymbol{w}||_2^2$$

$$\boldsymbol{w} = (\underbrace{\boldsymbol{\Phi}^T \boldsymbol{\Phi}}_{I^D \times I^D})^{-1}\ \boldsymbol{\Phi}^T\ \boldsymbol{y}$$

Assumptions:

- $N \geq I^D$
- Persistency of excitation: $\operatorname{rank}(\boldsymbol{\Phi}) = I^D$

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What if $\mathrm{rank}(\mathbf{\Phi}) < I^D$?

Kernel ridge regression

$$\min_{\boldsymbol{w}} ||\boldsymbol{y} - \mathbf{\Phi}\ \boldsymbol{w}||_2^2 + \lambda\ ||\boldsymbol{w}||_2^2$$

$$\boldsymbol{w} = (\mathbf{\Phi}^T\mathbf{\Phi} + \lambda\ \boldsymbol{I})^{-1}\ \mathbf{\Phi}^T\ \boldsymbol{y}$$

A simple example

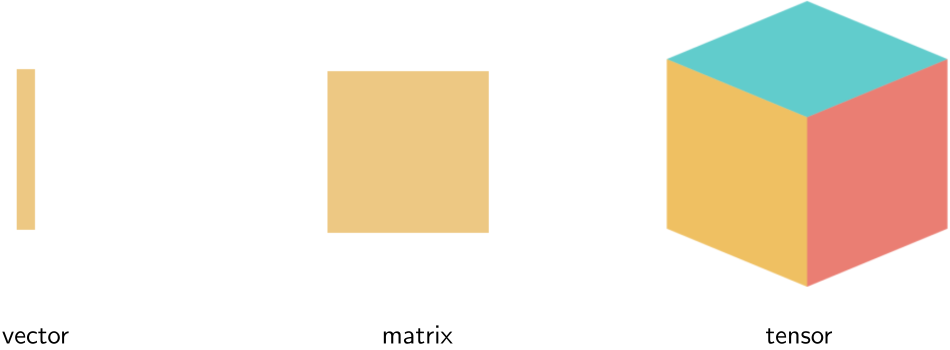
- $D = 18$ variables $x_1, \ldots, x_{18}$
- $I = 20$ basis functions
- $\boldsymbol{w}$ has $20^{18} = 2.6\ 10^{23}$ entries $\approx 10^{10}$ ChatGPTs

Tensor networks allow you to efficiently solve

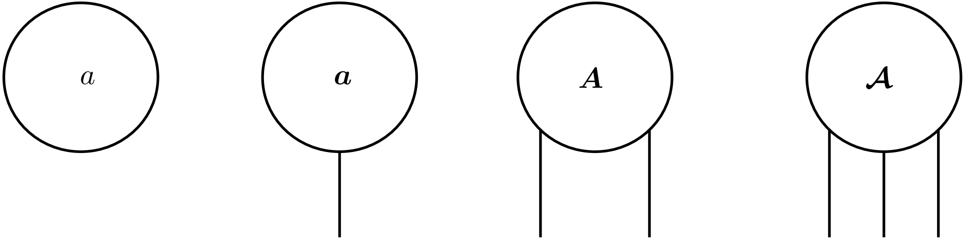
$$\left(\mathbf{\Phi}^T \mathbf{\Phi} + \boldsymbol{P}\right) \boldsymbol{w} = \mathbf{\Phi}^T \boldsymbol{y}$$

without explicitly making / inverting $(\mathbf{\Phi}^T \mathbf{\Phi} + \boldsymbol{P})$.

A tensor is a high-dimensional generalization of vectors and matrices

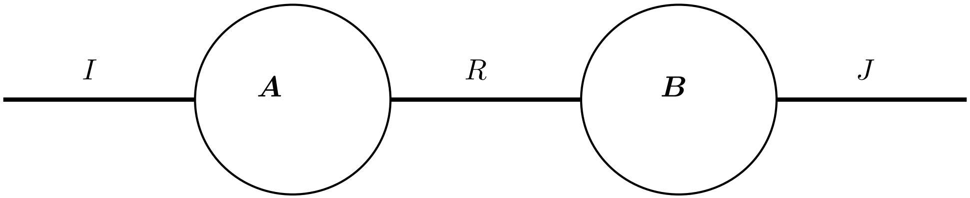


Tensor diagrams



Index summation is visualized as a common edge

$$\boldsymbol{C}(i,j) = \sum_{r=1}^{R} \boldsymbol{A}(i,r)\ \boldsymbol{B}(r,j)$$



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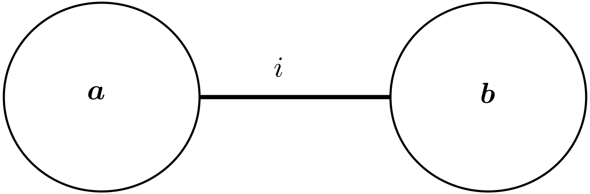
Brain teaser



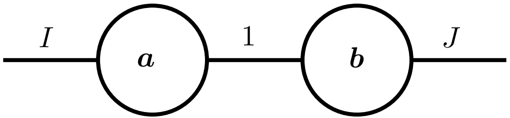
inner product: $\sum_{i=1}^{I} \boldsymbol{a}(i)\, \boldsymbol{b}(i) = \boldsymbol{a}^T \boldsymbol{b}$

An important operation: Outer product of vector $\boldsymbol{a}$ with vector $\boldsymbol{b}$

$$\boldsymbol{C} = \boldsymbol{a}\,\boldsymbol{b}^T = \boldsymbol{a} \circ \boldsymbol{b}$$

$$\boldsymbol{C}(i,j) = \boldsymbol{a}(i)\ \ \boldsymbol{b}(j)$$

$$\boldsymbol{C}(i,j) = \sum_{r=1}^{1} \boldsymbol{a}(i,r)\ \boldsymbol{b}(r,j)$$



Key idea

Replacing $\mathbf{\Phi}, \boldsymbol{P}, \boldsymbol{w}$ by networks of much smaller tensors avoids explicit construction/inversion of $\mathbf{\Phi}, \boldsymbol{P}, \boldsymbol{w}$ and enables efficient learning.

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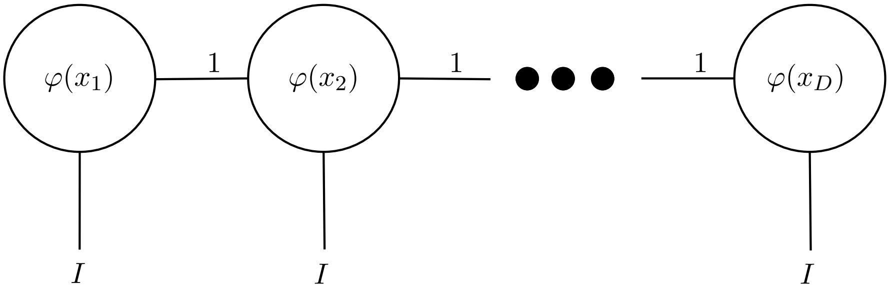
Back to our kernel machines

$$\boldsymbol{\phi} = \varphi(x_1) \circ \varphi(x_2) \circ \cdots \circ \varphi(x_D)$$



$$I^D \rightarrow D\, I$$

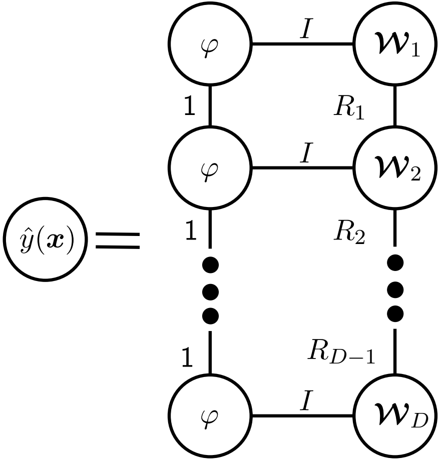
Revisit bivariate monomial basis functions as a tensor product

$$\boldsymbol{\phi} = \varphi(x_1) \circ \varphi(x_2)$$

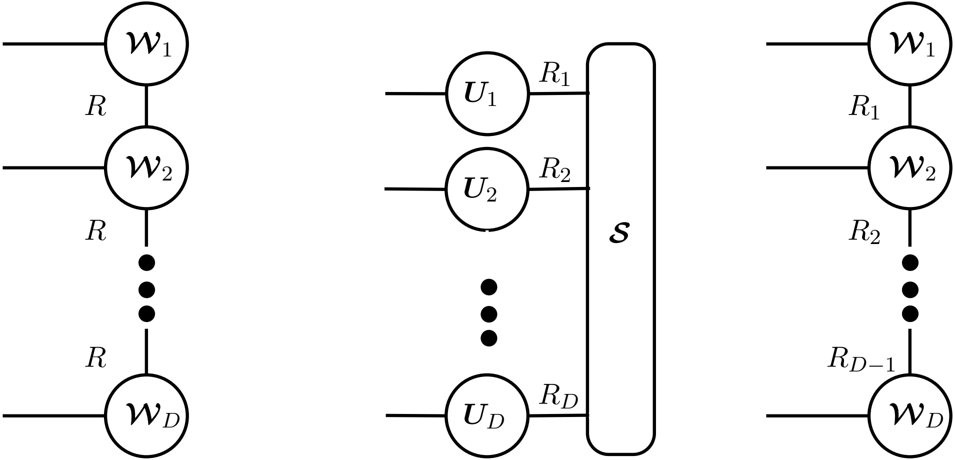
$$\begin{pmatrix} 1 & x_2 & x_2^2 \\ x_1 & x_1 x_2 & x_1 x_2^2 \\ x_1^2 & x_1^2 x_2 & x_1^2 x_2^2 \end{pmatrix} = \begin{pmatrix} 1 \\ x_1 \\ x_1^2 \end{pmatrix} \circ \begin{pmatrix} 1 \\ x_2 \\ x_2^2 \end{pmatrix}$$

Tensor-based kernel machine

$$y = \langle \boldsymbol{\phi}, \boldsymbol{\mathcal{W}} \rangle + e$$



Possible tensor network topologies...



Polyadic
DIR

Tucker
$R^D + DIR$

Tensor Train
DIR^2

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From linear least-squares to nonlinear least-squares

$$\min_{\mathcal{W}_1,\mathcal{W}_2,\ldots,\mathcal{W}_D} ||\boldsymbol{y}-\langle \boldsymbol{\phi},\ \mathrm{TN}(\mathcal{W}_1,\mathcal{W}_2,\ldots,\mathcal{W}_D)\rangle||_2^2\ +\ R(\mathrm{TN}(\mathcal{W}_1,\mathcal{W}_2,\ldots,\mathcal{W}_D))$$

Solving a polynomial system of equations!

Exploiting tensor network structure enables efficient learning

$\mathrm{TN}(\mathcal{W}_1, \mathcal{W}_2, \ldots, \mathcal{W}_D)$ is a linear map in $\mathcal{W}_1$

$$\mathrm{TN}(\mathcal{W}_1, \mathcal{W}_2, \ldots, \mathcal{W}_D) \rightarrow \mathrm{TN}_1(\mathcal{W}_1) = \boldsymbol{T}_1 \, \boldsymbol{w}_1$$

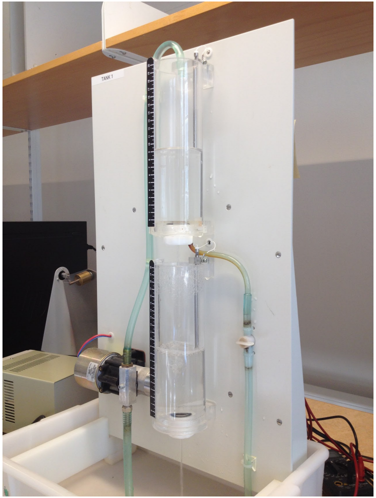
$$\min_{\boldsymbol{w}_1} ||\boldsymbol{y} - \boldsymbol{\Phi} \, \boldsymbol{T}_1 \, \boldsymbol{w}_1||_2^2 \, + \, \mathcal{R}(\boldsymbol{T}_1 \, \boldsymbol{w}_1)$$

Computational cost polyadic network: $O\left(N(IR)^2 + (IR)^3\right)$

Example: Cascaded tanks

- u_n : pump voltage
- y_n : water level lower tank
- Task: learn

$$\hat{y}_n\left(u_{n-1}, u_{n-2}, \ldots, y_{n-1}, y_{n-2}, \ldots\right)$$



Example: SUSY binary classification problem

$I = 20, D = 18, N = 5,000,000$

	AUC		1-Accuracy (%)	Time (s)
Technique	Low-level	Complete	Complete	Complete
BDT	0.850 ± 0.003	0.863 ± 0.003	NA	NA
NN	0.867 ± 0.002	0.875 ± 0.001	NA	NA
Dropout NN	0.856 ± 0.001	0.873 ± 0.001	NA	NA
DNN	0.872 ± 0.001	0.876 ± 0.001	NA	NA
Dropout DNN	$\mathbf{0.876 \pm 0.001}$	$\mathbf{0.879 \pm 0.001}$	NA	NA
VISH	0.859 ± 0.001	NA	NA	NA
CPD-SIP $(R = 5)$	0.860 ± 0.001	0.871 ± 0.001	20.14 ± 0.04	1416 ± 12
CPD-SIP $(R = 10)$	0.869 ± 0.001	0.872 ± 0.002	19.97 ± 0.10	3567 ± 1
CPD-SIP $(R = 15)$	0.871 ± 0.001	0.873 ± 0.001	19.86 ± 0.10	5628 ± 153
CPD-SIP $(R = 20)$	0.872 ± 0.001	0.875 ± 0.001	19.74 ± 0.04	9437 ± 721

References

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