KU LEUVEN

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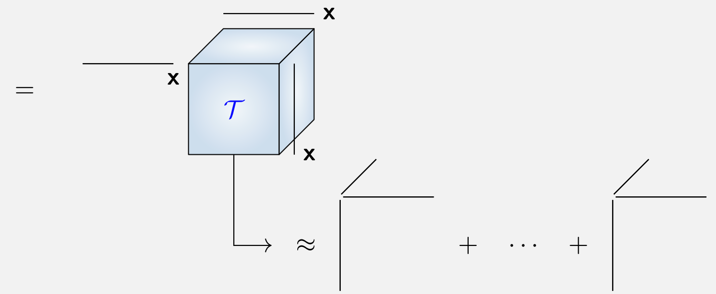
For more information:

Scalable multivariate polynomial regression by breaking the curse of dimensionality using tensor models

Thesis abstract: Tensor-based pattern recognition, data analysis and learning

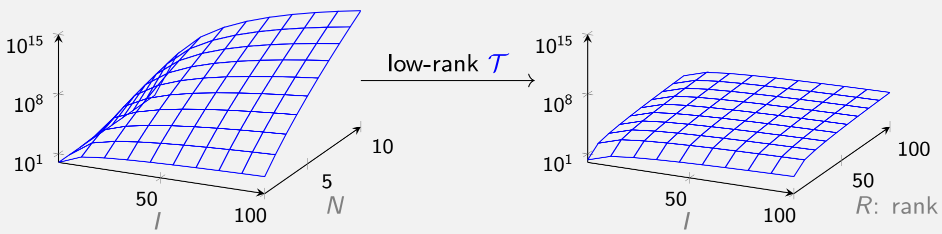
We achieve our goal, namely scalable multivariate polynomial regression, by approximating the polynomial coefficients with a **low-rank tensor**, which greatly reduces the amount of model parameters. For example, modeling the Gibbs free energy $G(\mathbf{x})$ of a metal alloy:

$$G(\mathbf{x}) \approx p(\mathbf{x}) = t_1 x_1^3 + t_2 x_1^2 x_2 + t_3 x_1 x_2^2 + t_4 x_2^3 \quad \text{with} \quad \mathbf{x} = \begin{bmatrix} x_1 & x_2 \end{bmatrix}^\top$$

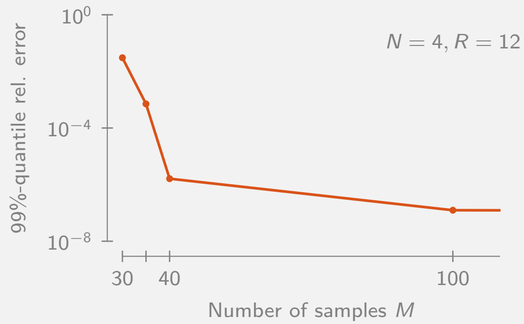


Contribution: The amount of coefficients of a multivariate polynomial $p(\mathbf{x})$ depends exponentially on its degree N and the amount of variables I. We **break the curse of dimensionality** with a low-rank coefficient tensor, which allows us to develop scalable algorithms.

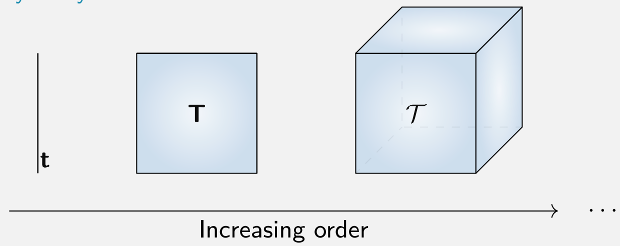
$p(\mathbf{x})$ #param $= \frac{(I+N-1)!}{N!(I-1)!}$ $\qquad$ $p(\mathbf{x})$ #param $= R(I+1)$



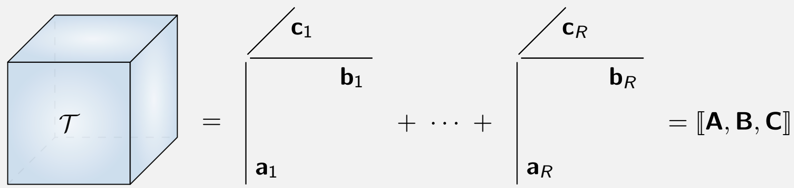
Application: This model accurately estimates the Gibbs free energy of a metal alloy, while only requiring few training data points.



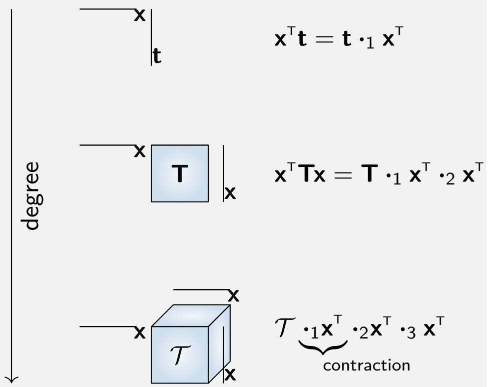
While vectors and matrices represent one- and two-way data arrays, higher-order tensors represent multi-way arrays of data.



Like matrices, tensors admit low-rank models that can represent data in a compact way.



Link: A multivariate polynomial can be rewritten with a higher-order symmetric tensor containing its coefficients.



Although we only consider homogeneous polynomials, we can easily extend to non-homogeneous polynomials through a process called homogenization.

By generalizing linear regression to a higher degree and more variables, we obtain a more expressive model.