Beating the Perils of Non-Convexity: Training Neural Networks using Tensor Methods

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Joint work with Majid Janzamin and Hanie Sedghi.

U.C. Irvine

Learning with Big Data

- High dimensional regime: as data grows, more variables!
- Useful information: low-dimensional structures.
- Learning with big data: ill-posed problem.

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Learning is finding needle in a haystack

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Learning is finding needle in a haystack

- Learning with big data: statistically and computationally challenging!

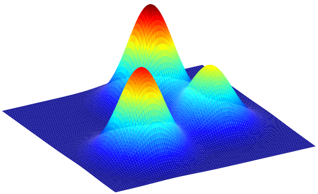
Optimization for Learning

Most learning problems can be cast as optimization.

Unsupervised Learning

- Clustering
  k-means, hierarchical ...

- Maximum Likelihood Estimator
  Probabilistic latent variable models

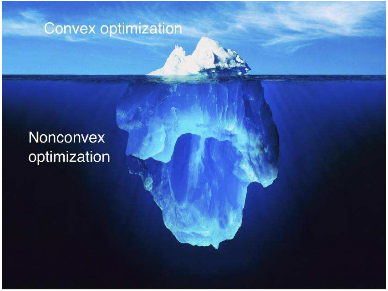


Supervised Learning

- Optimizing a neural network wrt a loss function

Convex vs. Non-convex Optimization

Progress is only tip of the iceberg..



Images taken from https://www.facebook.com/nonconvex

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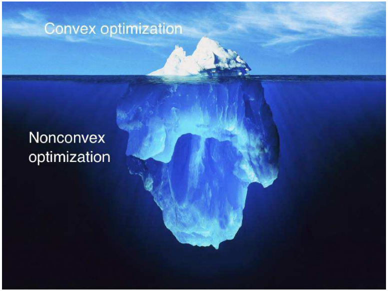
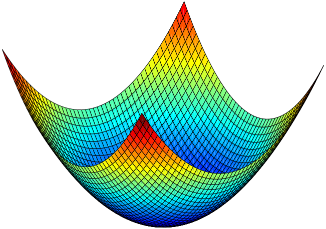
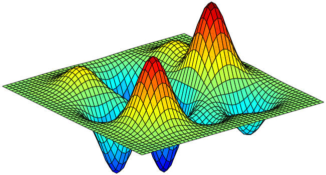


Real world is mostly non-convex!

Images taken from `https://www.facebook.com/nonconvex`

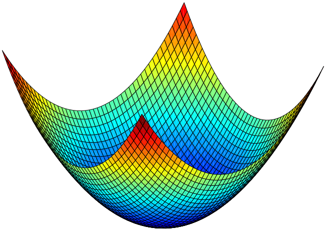
Convex vs. Nonconvex Optimization

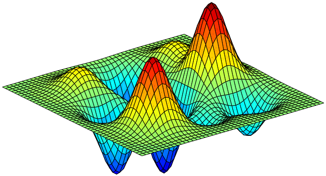




- One global optima.
- Multiple local optima

Convex vs. Nonconvex Optimization





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- Multiple local optima
- In high dimensions possibly exponential local optima

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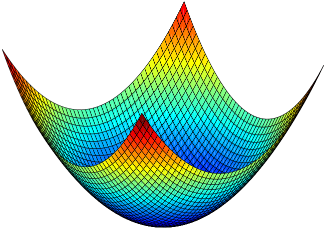

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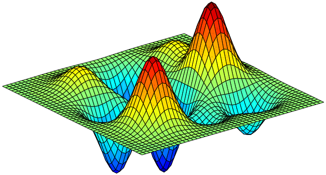

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How to deal with non-convexity?

Agenda

Beating the Perils of Non-Convexity:

Guaranteed Training of Neural Networks using Tensor Methods

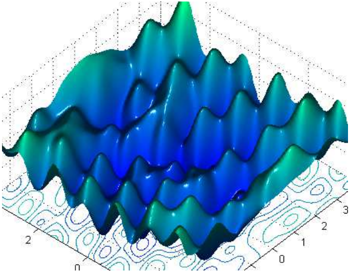
Recent Breakthroughs in Tensor Methods

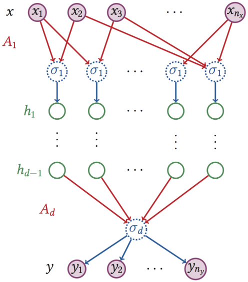
Overcomplete models, Convolutional models, Reinforcement Learning of POMDPs . . .

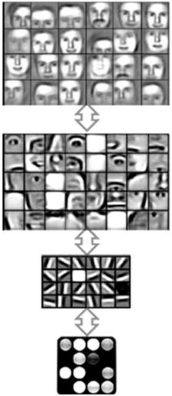
Outline

Training Neural Networks

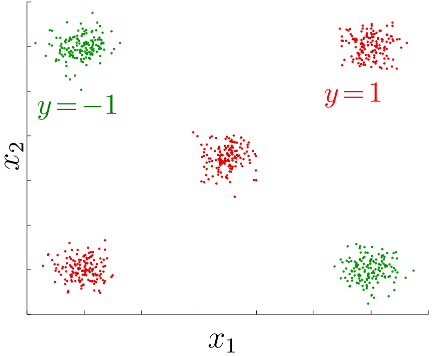
- Tremendous practical impact with deep learning.
- Algorithm: backpropagation.
- Highly non-convex optimization



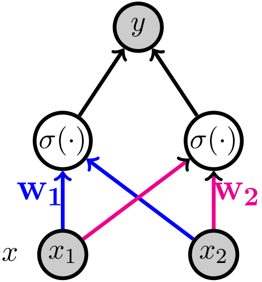




Toy Example: Failure of Backpropagation



Labeled input samples
Goal: binary classification

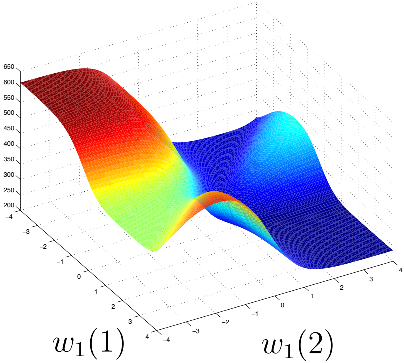


Our method: guaranteed risk bounds for training neural networks

Backpropagation vs. Our Method

Weights w_2 randomly drawn and fixed

Backprop (quadratic) loss surface



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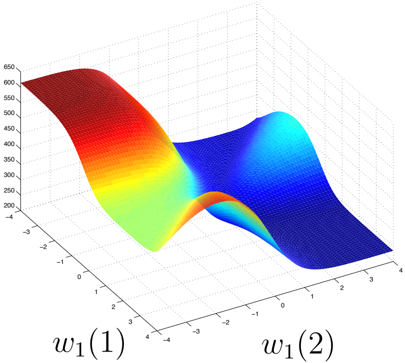
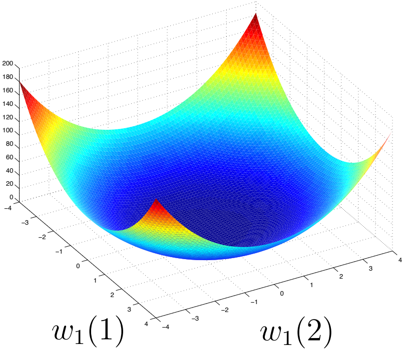


Loss surface for our method



Previous Results on Training Neural Networks

Risk bounds (for computationally hard algorithms)

- Approximation bounds for neural networks. *Barron '90.*
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Computational complexity

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Gradient descent/ Local search

- No spurious local optima for linear networks. *Baldi & Hornik '89.*
- Failure cases: manifold of spurious local optima. *Frasconi et al. '97.*
- Random (first layer) weights suffice for polynomials under Gaussian input. *Andoni et. al. '14.*
- Incremental training with polynomial activations. *Livni et al. '14.*

Alternatives to gradient descent: computationally efficient with guarantees?

Overcoming Hardness of Training

In general, training a neural network is NP hard.

How does knowledge of input distribution help?

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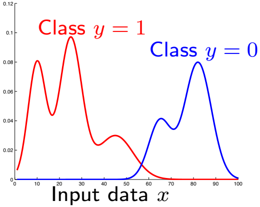
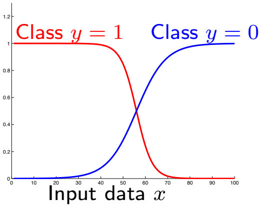
Generative vs. Discriminative Models

$p(x, y)$



$p(y|x)$

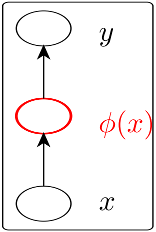


- Generative models: Encode domain knowledge.
- Discriminative: good classification performance.
- Neural Network is a discriminative model.

Feature Transformation for Training Neural Networks

Feature learning: Learn $\phi(\cdot)$ from input data.

How to use $\phi(\cdot)$ to train neural networks?



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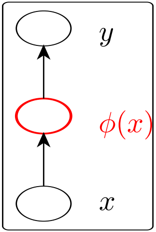


Multivariate Moments: Many possibilities, ...

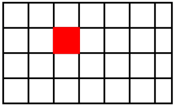
$$\mathbb{E}[x \otimes y], \quad \mathbb{E}[x \otimes x \otimes y], \quad \mathbb{E}[\phi(x) \otimes y], \quad \ldots$$

Tensor Notation for Higher Order Moments

- Multi-variate higher order moments form tensors.
- Are there spectral operations on tensors akin to PCA on matrices?

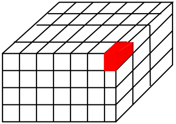
Matrix

- $\mathbb{E}[x \otimes y] \in \mathbb{R}^{d \times d}$ is a second order tensor.
- $\mathbb{E}[x \otimes y]_{i_1,i_2} = \mathbb{E}[x_{i_1} y_{i_2}]$.
- For matrices: $\mathbb{E}[x \otimes y] = \mathbb{E}[xy^\top]$.



Tensor

- $\mathbb{E}[x \otimes x \otimes y] \in \mathbb{R}^{d \times d \times d}$ is a third order tensor.
- $\mathbb{E}[x \otimes x \otimes y]_{i_1,i_2,i_3} = \mathbb{E}[x_{i_1} x_{i_2} y_{i_3}]$.

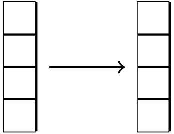


- In general, $\mathbb{E}[\phi(x) \otimes y]$ is a tensor.
- What class of $\phi(\cdot)$ useful for training neural networks?

Score Function Transformations

- Score function for $x \in \mathbb{R}^d$ with pdf $p(\cdot)$:

$$\boxed{\mathcal{S}_1(x) := -\nabla_x \log p(x)}$$



Input: $x \in \mathbb{R}^d$ $\qquad$ $\mathcal{S}_1(x) \in \mathbb{R}^d$

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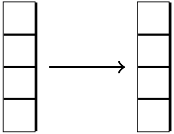
$$\boxed{\mathcal{S}_m(x) := (-1)^m \frac{\nabla^{(m)} p(x)}{p(x)}}$$



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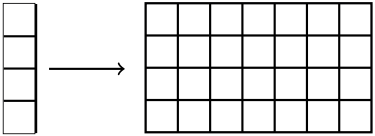

Input: $x \in \mathbb{R}^d$

$\mathcal{S}_2(x) \in \mathbb{R}^{d \times d}$

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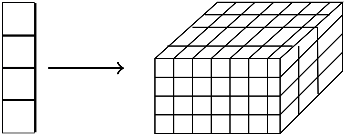


Input: $x \in \mathbb{R}^d$

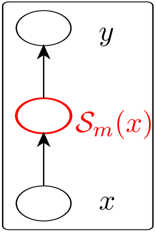
$\mathcal{S}_3(x) \in \mathbb{R}^{d \times d \times d}$

Why score functions?

- Higher order score function:

$$\boxed{\mathcal{S}_m(x) := (-1)^m \frac{\nabla^{(m)} p(x)}{p(x)}}$$

- Form the cross-moments: $\mathbb{E}\left[y \otimes \mathcal{S}_m(x)\right]$.



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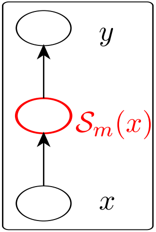


Theorem (Score function property, JSA'14)

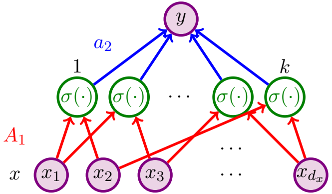
- Providing derivative information: let $\mathbb{E}[y|x] := f(x)$, then

$$\mathbb{E}\left[y \otimes \mathcal{S}_m(x)\right] = \mathbb{E}\left[\nabla_x^{(m)} f(x)\right].$$

"Score Function Features for Discriminative Learning: Matrix and Tensor Framework" by M. Janzamin, H. Sedghi, and A. , Dec. 2014.

Moments of a Neural Network

$$\mathbb{E}[y|x] = G(x) = a_2^\top \sigma(A_1^\top x + b_1) + b_2$$



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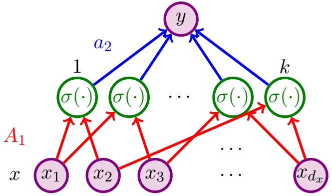

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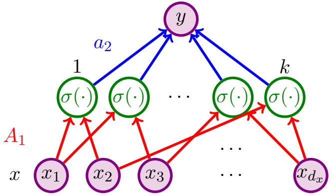

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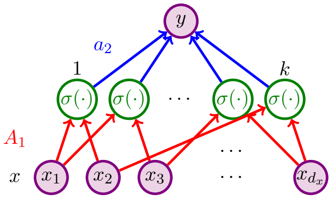

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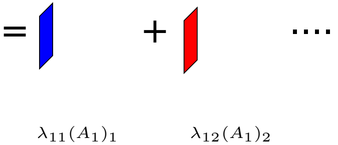

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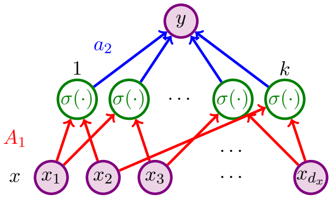

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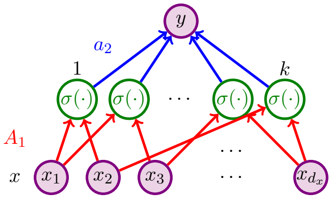

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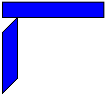
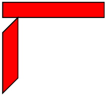
=  +  ····

$\lambda_{11}(A_1)_1 \otimes (A_1)_1$ $\lambda_{12}(A_1)_2 \otimes (A_1)_2$

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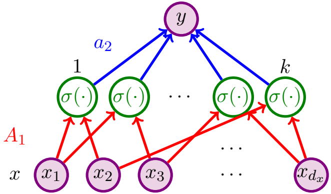

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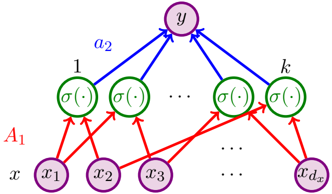

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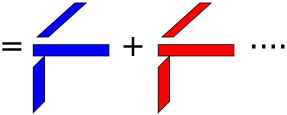

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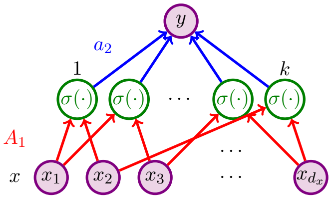

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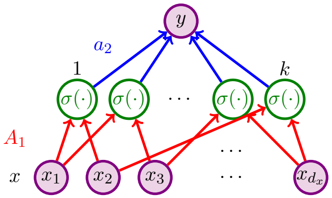
Why tensors are required?

- Matrix decomposition recovers subspace, not actual weights.
- Tensor decomposition uniquely recovers under non-degeneracy.

Moments of a Neural Network

$$\boxed{\mathbb{E}[y|x] = G(x) = a_2^\top \sigma(A_1^\top x + b_1) + b_2}$$



- Given labeled examples $\{(x_i, y_i)\}$

$$\mathbb{E}\left[y \cdot \mathcal{S}_m(x)\right] = \mathbb{E}\left[\nabla^{(m)} G(x)\right]$$

$$\Downarrow$$

$$\boxed{M_3 = \mathbb{E}[y \cdot \mathcal{S}_3(x)] = \sum_{j \in [k]} \lambda_{3,j} \cdot (A_1)_j \otimes (A_1)_j \otimes (A_1)_j}$$

- Guaranteed learning of weights of first layer via tensor decomposition.
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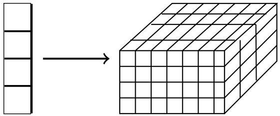
NN-LiFT: Neural Network LearnIng using Feature Tensors

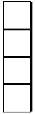


Input:
$x \in \mathbb{R}^d$

$\mathcal{S}_3(x) \in \mathbb{R}^{d \times d \times d}$

NN-LiFT: Neural Network LearnIng using Feature Tensors

Estimating M_3 using
labeled data $\{(x_i, y_i)\}$



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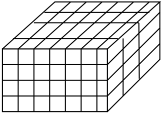
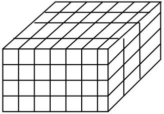


$\mathcal{S}_3(x) \in \mathbb{R}^{d\times d\times d}$

Cross-moment

$$\xrightarrow{\text{Cross-moment}} \frac{1}{n}\sum_{i=1}^{n} y_i \otimes \mathcal{S}_3(x_i) = \frac{1}{n}\sum_{i=1}^{n} y_i \otimes$$



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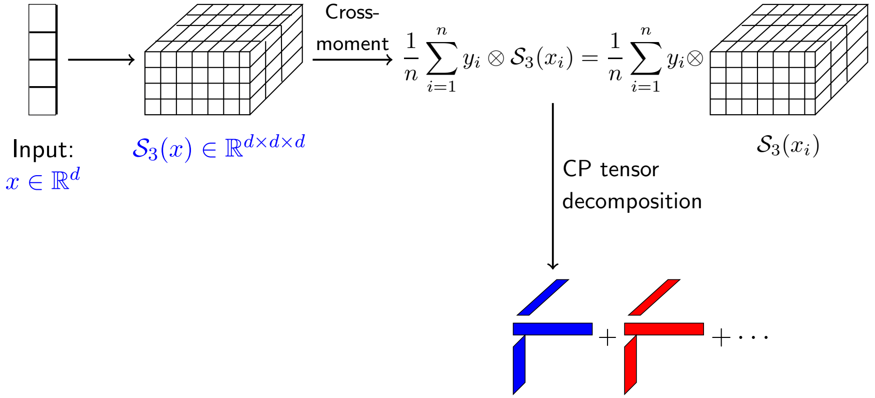

Rank-1 components are the estimates of columns of A_1

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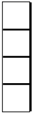
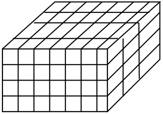
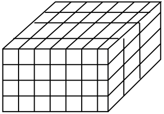
 $\longrightarrow$  $\xrightarrow{\text{Cross-moment}}$ $\displaystyle \frac{1}{n}\sum_{i=1}^{n} y_i \otimes \mathcal{S}_3(x_i) = \frac{1}{n}\sum_{i=1}^{n} y_i \otimes$ 

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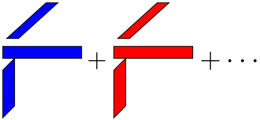
CP tensor decomposition



Rank-1 components are the estimates of columns of A_1

Fourier technique $\Rightarrow a_2, b_1, b_2$

Estimation error bound

- Guaranteed learning of weights of first layer via tensor decomposition.

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Rank-1 tensor: $T = w \cdot a \otimes b \otimes c \Leftrightarrow T(i,j,l) = w \cdot a(i) \cdot b(j) \cdot c(l).$

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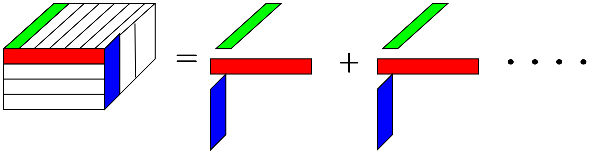

Tensor T $\qquad w_1 \cdot a_1 \otimes b_1 \otimes c_1 \qquad w_2 \cdot a_2 \otimes b_2 \otimes c_2$

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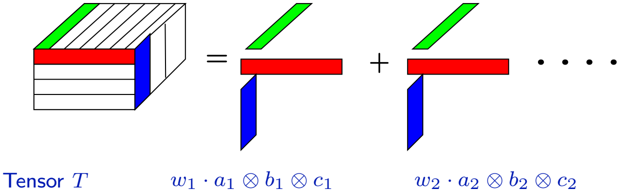

- Algorithm: Alternating Least Square (ALS), Tensor power iteration, ...

Orthogonal Tensor Power Method

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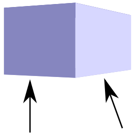

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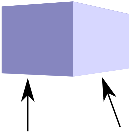

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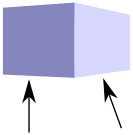

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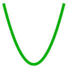

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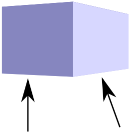

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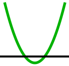

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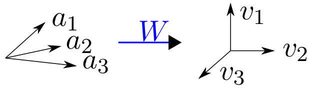
For an orthogonal tensor, no spurious local optima!

Guaranteed Tensor Decomposition

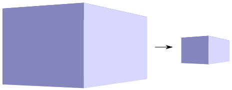
Undercomplete tensors $(k \leq d)$ with full rank components

Non-orthogonal decomposition $T_1 = \sum_{i \in [k]} \lambda_i a_i \otimes a_i \otimes a_i$.

- Whitening matrix W: computed from tensor slices.



- Multilinear transform: $T_2 = T_1(W, W, W)$ to orthogonalize.



Tensor T_1 Tensor T_2

- To do whitening we need A_1 to be full column rank.

How to handle $k > d$?

Flatten higher order tensor to third order so that full rank condition holds, e.g. using 6^{th} order moments, we can handle $k = o(d^2)$.

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---

- Known: continuous functions with compact domain can be arbitrarily well approximated by neural networks with one hidden layer.

Approximation Error

- Approx. error related to Fourier spectrum of $f(x)$. (*Barron '93*).
$$\mathbb{E}[y|x] = f(x)$$

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$$F(\omega) := \int_{\mathbb{R}^d} f(x) e^{-j\langle\omega,x\rangle} dx$$

$$C_f := \int_{\mathbb{R}^d} \|\omega\|_2 \cdot |F(\omega)| d\omega$$

Approximation error $\leq C_f/\sqrt{k}$

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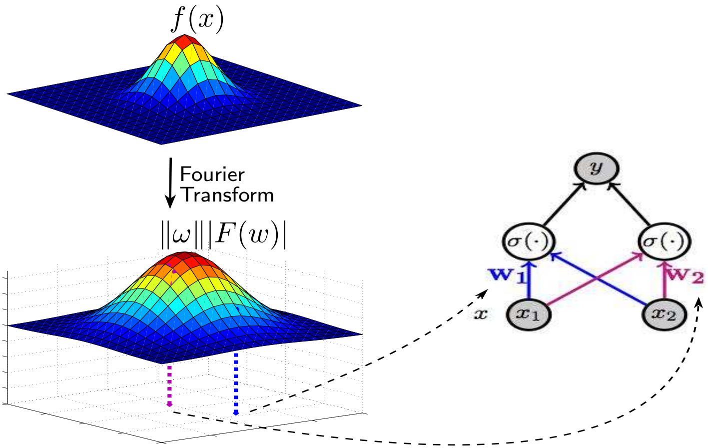

Our Main Result: Risk Bounds

- Approximating arbitrary function $f(x)$ with bounded

$$C_f := \int_{\mathbb{R}^d} \|\omega\|_2 \cdot |F(\omega)| d\omega$$

- n samples, d input dimension, k number of neurons.

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Theorem(JSA'14)

- Assume C_f is small.

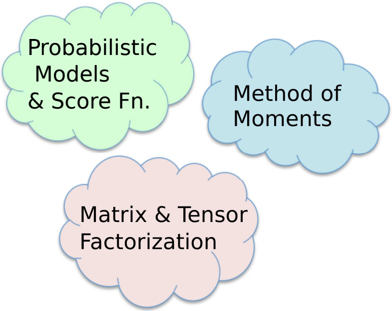
$$\mathbb{E}[|f(x) - \hat{f}(x)|^2] \leq O(C_f^2/k) + O(1/n).$$

- Polynomial sample complexity n in terms of dimensions d, k.
- Computational complexity same as SGD with enough parallel processors.

"Beating the Perils of Non-Convexity: Guaranteed Training of Neural Networks using Tensor Methods" by M. Janzamin, H. Sedghi and A. , June. 2015.

FEAST: Feature ExtrAction using Score function Tensors

- Mixture of generalized linear models (SA'14)
  - The first framework to learn the weight vectors instead of their subspace.
- Mixture of Linear Regression



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- Mixture of Linear Regression
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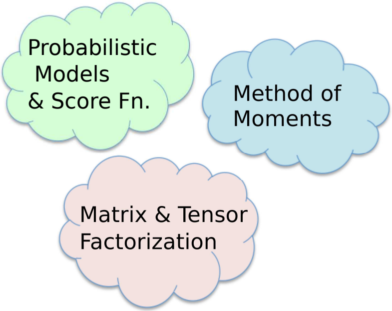
- Recurrent Neural Networks



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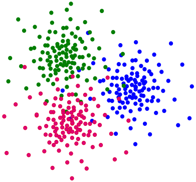
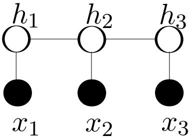
Outline

Tractable Learning for LVMs

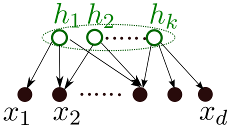
GMM



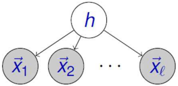
HMM



ICA



Multiview and Topic Models



$h \in [k]$,

$\vec{x}_1 \in \mathbb{R}^{d_1}, \vec{x}_2 \in \mathbb{R}^{d_2}, \ldots, \vec{x}_\ell \in \mathbb{R}^{d_\ell}$.

$k = \#$ components, $\ell = \#$ views (*e.g.*, audio, video, text).

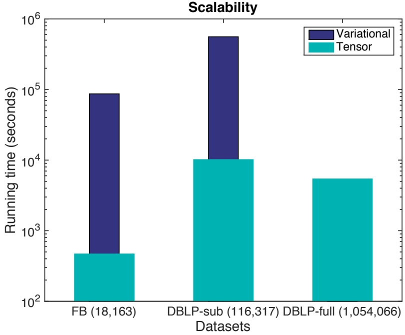
View 1: $\vec{x}_1 \in \mathbb{R}^{d_1}$

View 2: $\vec{x}_2 \in \mathbb{R}^{d_2}$

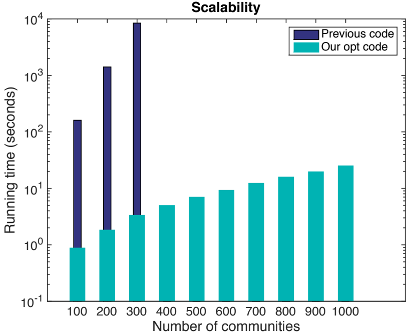
View 3: $\vec{x}_3 \in \mathbb{R}^{d_3}$

Results for Community Detection

Tensor vs. Variational



Our Tensor Code



At Scale Tensor Computations

Randomized Tensor Sketches

- Naive computation scales exponentially in order of the tensor.
- Propose randomized FFT sketches.
- Computational complexity independent of tensor order.
- Linear scaling in input dimension and number of samples.

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(1) *Fast and Guaranteed Tensor Decomposition via Sketching* by Yining Wang, Hsiao-Yu Tung, Alex Smola, A. , NIPS 2015.

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Tensor Contractions with Extended BLAS Kernels on CPU and GPU

- BLAS: Basic Linear Algebraic Subprograms, highly optimized libraries.
- Use extended BLAS to minimize data permutation, I/O calls.

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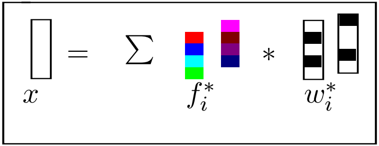
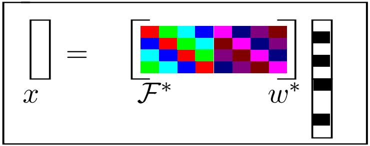
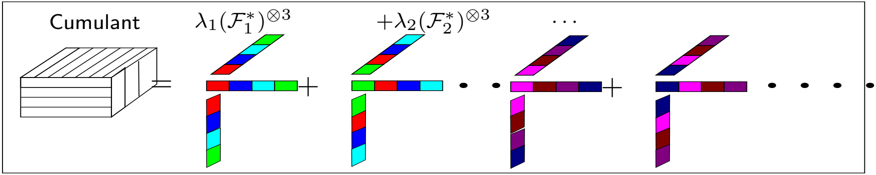
Convolutional Tensor Decomposition



(a) Convolutional dictionary model



(b) Reformulated model



Efficient methods for tensor decomposition with circulant constraints.

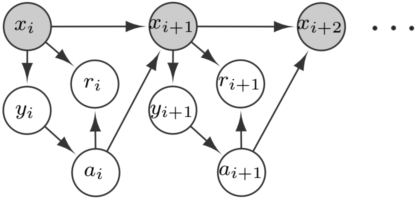
Convolutional Dictionary Learning through Tensor Factorization by F. Huang, A. , June 2015.

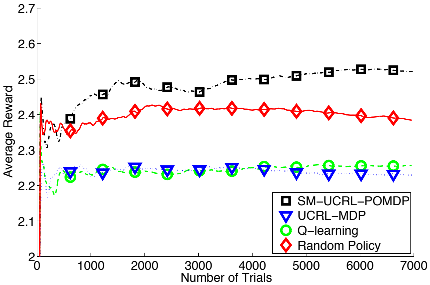
Reinforcement Learning (RL) of POMDPs

- Partially observable Markov decision processes.

Proposed Method

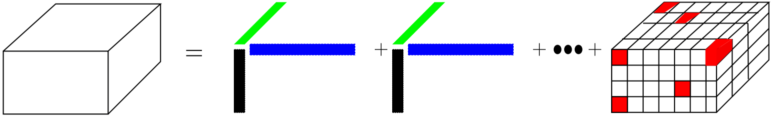
- Consider memoryless policies. Episodic learning: indirect exploration.
- Tensor methods: careful conditioning required for learning.
- First RL method for POMDPs with logarithmic regret bounds.





Logarithmic Regret Bounds for POMDPs using Spectral Methods by K. Azzizade, A. Lazaric, A.
, under preparation.

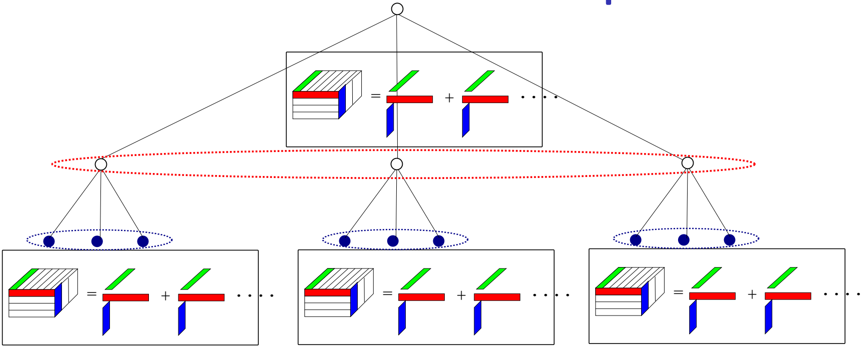
Sparse+Low Rank Tensor Decomposition



- Decompose input tensor as low rank tensor + sparse tensor.
- Analyze convergence to global optimum for alternating projections (non-convex method)
- Power of tensor methods: Can handle much larger amount of block sparse perturbations than matrix methods applied to input tensor.

Robust tensor decomposition: Guarantees under block sparse perturbations by A. , U.N. Niranjan, Y. Shi, P. Jain, under preparation.

Hierarchical Tensor Decomposition

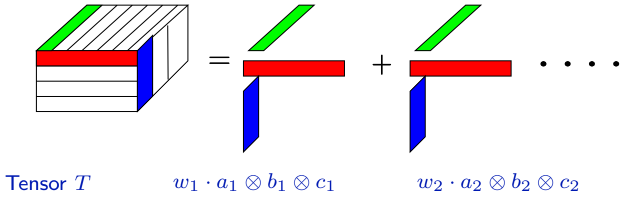


- Relevant for learning latent tree graphical models.
- Propose first algorithm for integrated learning of hierarchy and components of tensor decomposition.
- Highly parallelized operations but with global consistency guarantees.

Scalable Latent Tree Model and its Application to Health Analytics By F. Huang, U. N. Niranjan, J. Perros, R. Chen, J. Sun, A. , Preprint, June 2014.

Overcomplete Tensor Decomposition

$$\boxed{T = \sum_{j \in [k]} w_j a_j \otimes b_j \otimes c_j.}$$



- Overcomplete: Tensor rank larger than input dimension $(k > d)$.
- First guaranteed results for recovery under incoherent components.
- Tensor rank much higher than dimension: for third order, $k = o(d^{1.5})$.

Learning Overcomplete Latent Variable Models through Tensor Methods by A. , R. Ge, M. Janzamin, COLT 2015.

Outline

Summary and Outlook

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- Tensor methods: a powerful paradigm for guaranteed large-scale machine learning.
- First methods to provide provable bounds for training neural networks, many latent variable models (e.g HMM, LDA), POMDPs!

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Outlook

- Training multi-layer neural networks, models with invariances, reinforcement learning using neural networks . . .
- Unified framework for tractable non-convex methods with guaranteed convergence to global optima?

My Research Group and Resources

- Podcast/lectures/papers/software available at http://newport.eecs.uci.edu/anandkumar/