Non-negative Tensor Decompositions for Unsupervised Learning

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Western Washington University, Bellingham, WA

Nicholas Richardson

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THE UNIVERSITY OF BRITISH COLUMBIA

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The Setting
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- Do you have a lot of data?

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- A function that depends on many independent variables

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Tensor Decompositions are for you!

What is a Tension Decomposition?

Overview

1. Take your data array

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2. Select a model

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Overview

1. Take your data array
2. Select a model
3. Solve a block-convex minimization problem between your data and a sum-product of smaller sized arrays using block coordinate gradient decent but its not converging to reasonable values because you forgot to set a unique scaling for your factors so you settle for a sub-optimal solution by projecting onto a reasonable set

What is a Tensor Decomposition?

Overview

1. Take your data array
2. Select a model
3. Write it as a product of smaller arrays

Benefits

Overview

- Less storage than original data

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- Easy to implement optimization problems often converge to Nash Point
  - Minima $\implies$ critical point $\implies$ (local) Nash point
  - Some models have: critical point $\iff$ (global) Nash point
- No “training” required
- none or only a few hyperparameters to tune

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Models

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- Order-N tensor

$$\mathcal{Y} \in \mathbb{R}^{I_1 \times \cdots \times I_N}$$

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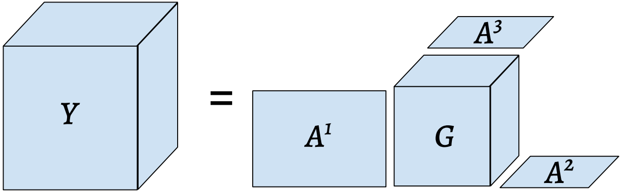
  - binary: $Y_{i_1 \ldots i_N} \in \{0, 1\}$
- If Y is too big to store, calculate $Y_{i_1 \ldots i_N}$ on-the-fly

Tucker Decomposition

Models

- Factorize Y into a core tensor $G \in \mathbb{R}^{R_1 \times \cdots \times R_N}$ and matrices $A^n \in \mathbb{R}^{I_n \times R_n}$



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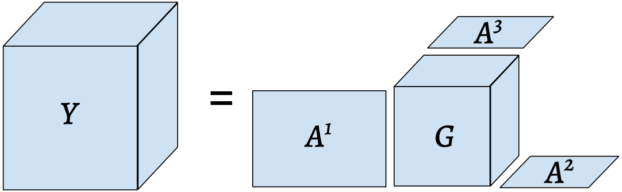

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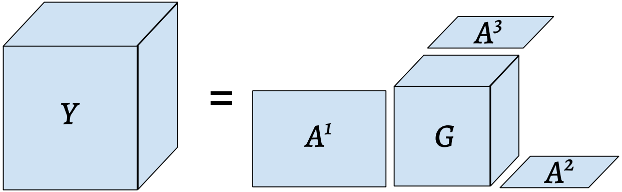
- Call Y a rank-$(R_1, \ldots, R_N)$ tensor, and R_n the n-rank where $R_n = \mathrm{rank}_n(Y)$



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- Tucker-n: $A^{n+1}, \ldots, A^N = I$ (possibly different sizes!)

$$Y = G \times_1 A^1 \times_2 \cdots \times_n A^n$$

$$\text{e.g. Tucker-1:} \quad Y = G \times_1 A$$

Extensions & Additional Compression

Models

- Factorize the core symmetrically (Extend Tucker)

$$G_{r_1 r_2 r_3} = \sum_{i,j,k=1}^{R} B^1_{r_1 jk} B^2_{i r_2 k} B^3_{ij r_3}$$

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- Tensor Trains (Extend Tucker-2)

$$Y_{i_1 \ldots i_N} = \sum_{r_1, r_N} A^1_{i_1 r_1} \underbrace{\sum_{j_2 \ldots j_{N-2}} A^2_{r_1 i_2 j_2} A^3_{j_2 i_3 j_3} \ldots A^{n-1}_{j_{N-2} i_{N-1} r_2}}_{G_{r_1 i_2 \ldots i_{N-1} r_N}} A^N_{i_N r_N}$$

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- Factorize the matrices (Extend CP)

$$A^n_{i_n r} = \sum_k T_{i_n rk} b_k$$

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  - $\displaystyle\sum_{i_1 \ldots i_N} Y_{i_1 \ldots i_N} \log \left(\frac{Y_{i_1 \ldots i_N}}{\hat{Y}_{i_1 \ldots i_N}} \right)$

Full Gradient Descent, Alternating Least-Squares, and Problems

Solving a model

- (Projected) Full Gradient Descent:

$$\mathcal{A} \leftarrow \arg\min_{\mathcal{B} \in C} \langle \nabla F(\mathcal{A}), \mathcal{B} - \mathcal{A} \rangle + \frac{1}{2\alpha} \|\mathcal{B} - \mathcal{A}\|_F^2$$

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$$A^n \leftarrow \arg\min_{A\in C} \|Y - f(A^1, \ldots, A^{n-1}, A, A^{n+1}, \ldots, A^N)\|_F^2$$

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  - may not converge to stationary point

Block Coordinate Descent (BCD)

Solving a model

- Combine into BCD:

$$A^n \leftarrow \arg\min_{A \in C} \langle \nabla_{A^n} F, A - A^n \rangle + \frac{1}{2\alpha} \|A - A^n\|_F^2$$

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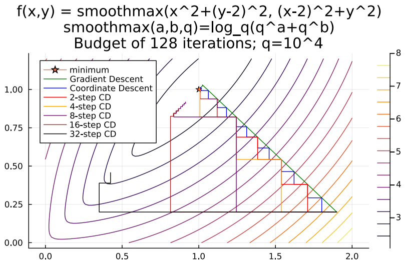

Figure: Full vs Coordinate Descent

Multiplicative Updates

Solving a model

- Alternate to BCD with non-negative constraint:

$$A^n_{i_1 \dots i_n} \leftarrow A^n_{i_1 \dots i_n} \beta^n_{i_1 \dots i_n} \quad \beta \geq 0$$

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- Ex: $F(A, B) = \frac{1}{2}\|Y - AB\|_F^2$ use

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- Ensures entries stay positive
- Equivalent to BCD with the stepsizes $\alpha^1_{ij} = \frac{A_{ij}}{(ABB^\top)_{ij}}$ and $\alpha^2_{ij} = \frac{B_{ij}}{(A^\top AB)_{ij}}$

Bells and Whistles

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- Line-search Stepsize:

$$\min_{\alpha > 0} F(A^1, \ldots, A^{n-1}, \underbrace{A^n - \alpha \nabla_{A^n} F}_{\text{line search}}, A^{n+1}, \ldots, A^N)$$

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Special Considerations

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Nash point condition

Let $F(\cdot, B), F(A, \cdot)$ be convex, and $(A_0, B_0) \in C = C_A \times C_B$ be point. Then,

$$\mathbf{0} \in \partial(F + \delta_C)(A_0, B_0) \iff \begin{array}{l} F(A_0, B_0) \leq F(A, B_0) \ \forall A \in C_A \\ F(A_0, B_0) \leq F(A_0, B) \ \forall B \in C_B \end{array}.$$

Selecting the Rank(s) R_n

Special Considerations

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- Option 2: When there's only 1 unknown rank;
  - Solve the model for all ranks $R = 1, \ldots, I$

$$R = \arg\max_{r} \kappa(r) := \frac{F''(r)}{(1 + F'(r)^2)^{1.5}}$$

Selecting the Rank(s) R_n

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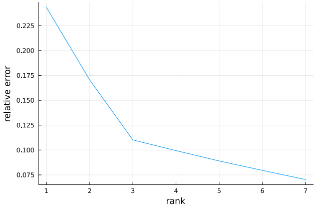
  - $R = 88$ since there are 88 keys
- Option 2: When there's only 1 unknown rank;
  - Solve the model for all ranks $R = 1, \ldots, I$
  - Compute final objective value $F(R)$

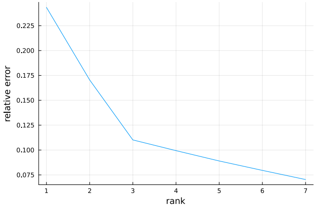


$$R = \arg\max_{r} \kappa(r) := \frac{F''(r)}{(1 + F'(r)^2)^{1.5}}$$

Selecting the Rank(s) R_n

Special Considerations

- Option 1: Use information about your physical system
  - e.g. decompose piano audio into notes and amplitudes
  - $R = 88$ since there are 88 keys
- Option 2: When there's only 1 unknown rank;
  - Solve the model for all ranks $R = 1, \ldots, I$
  - Compute final objective value $F(R)$
  - Select point of maximum curvature



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- Still only unique up to permutations of rows/columns/fibres

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References

Conclusion

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Thank you for listening!
Any questions?