Tensor Contraction with Extended BLAS Kernels on CPU and GPU

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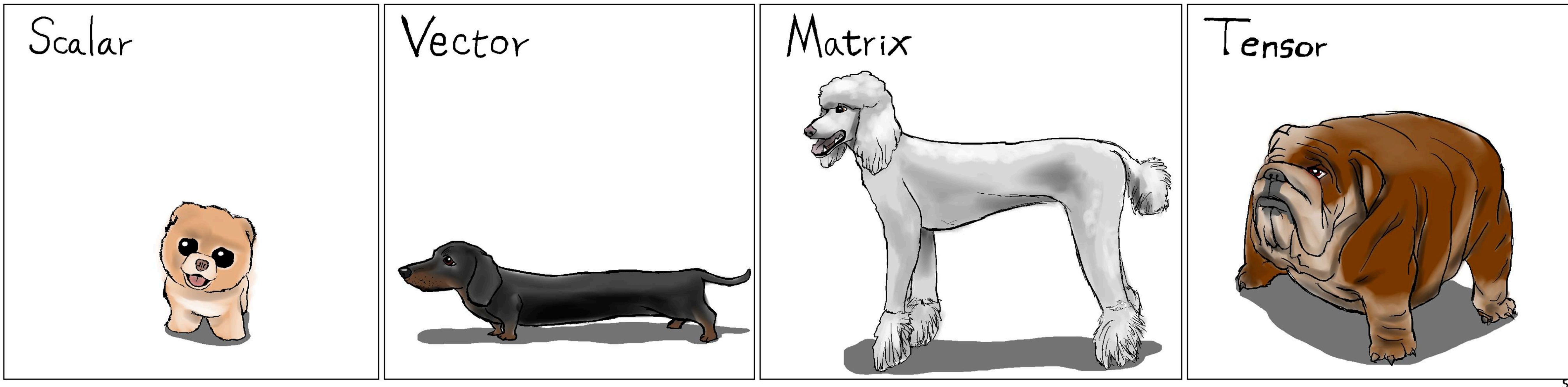
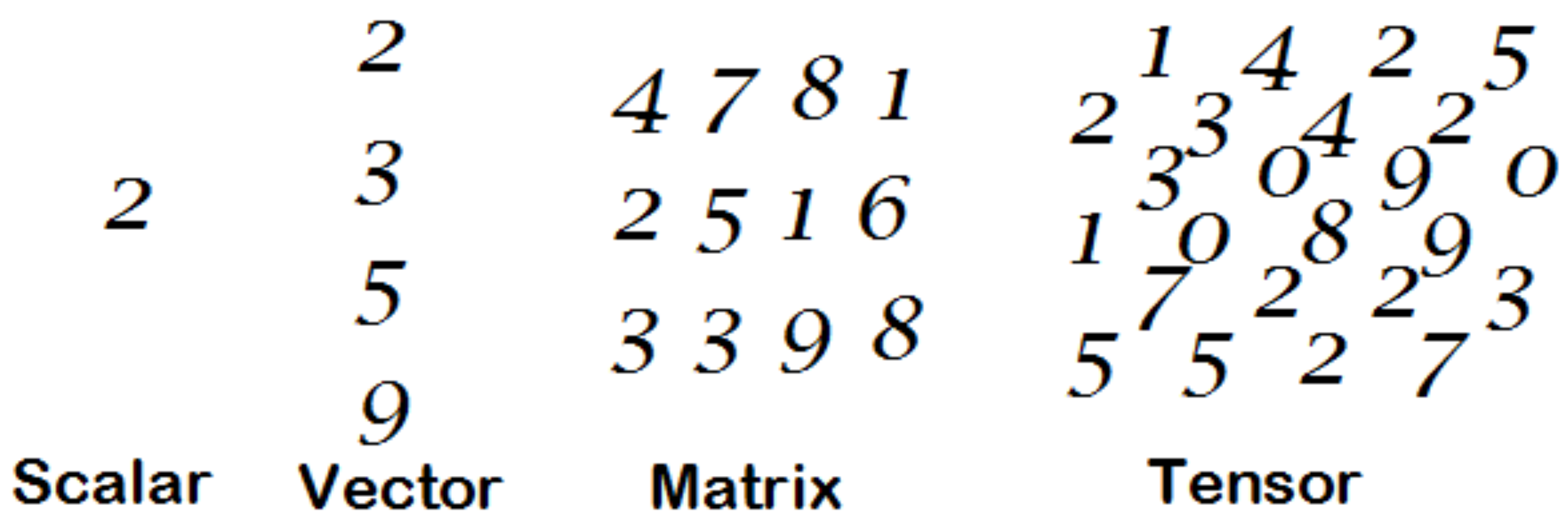
Joint work with U.N. Niranjan, Animashree Anandkumar and Cris Cecka

SIAM-ALA18

Tensor Contraction-Motivation





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Modern data is inherently multi-dimensional

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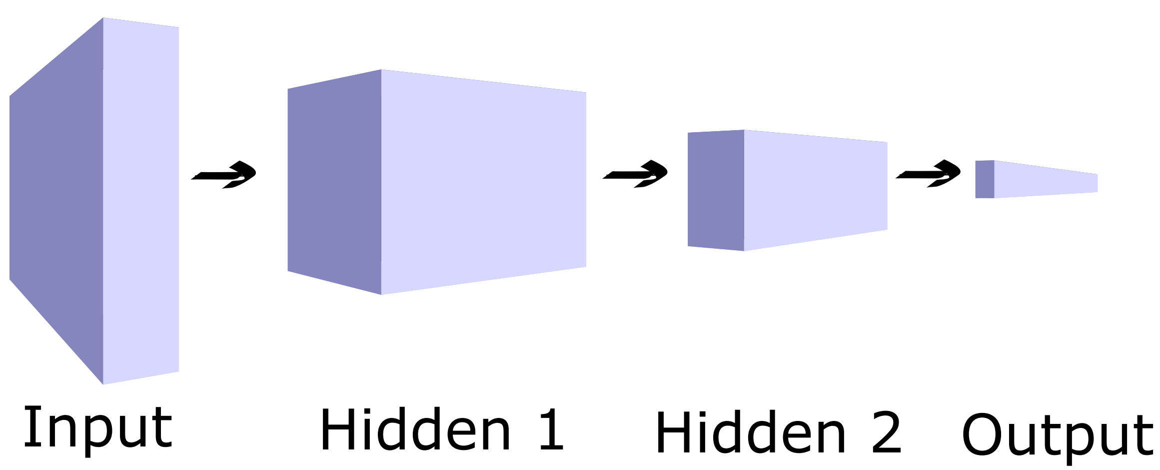
Neural Networks



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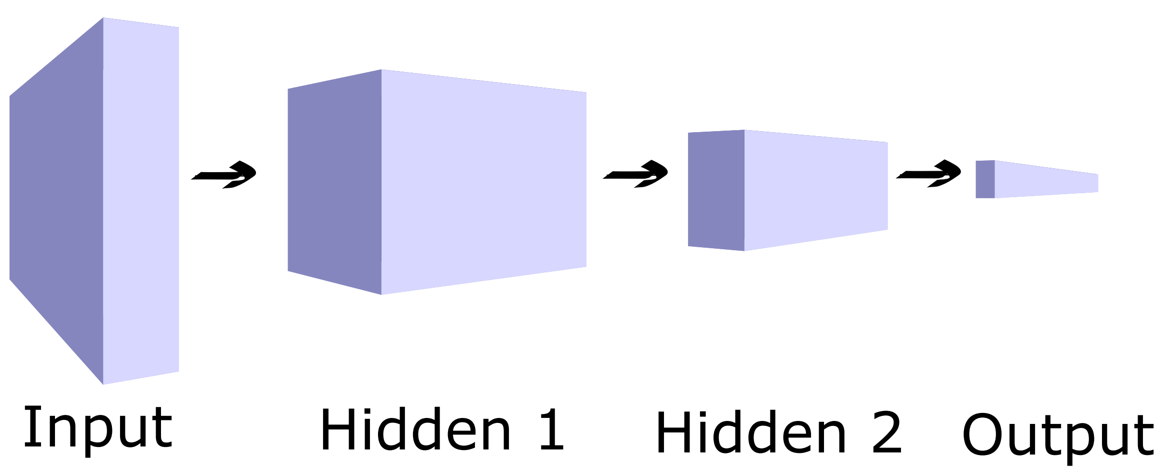
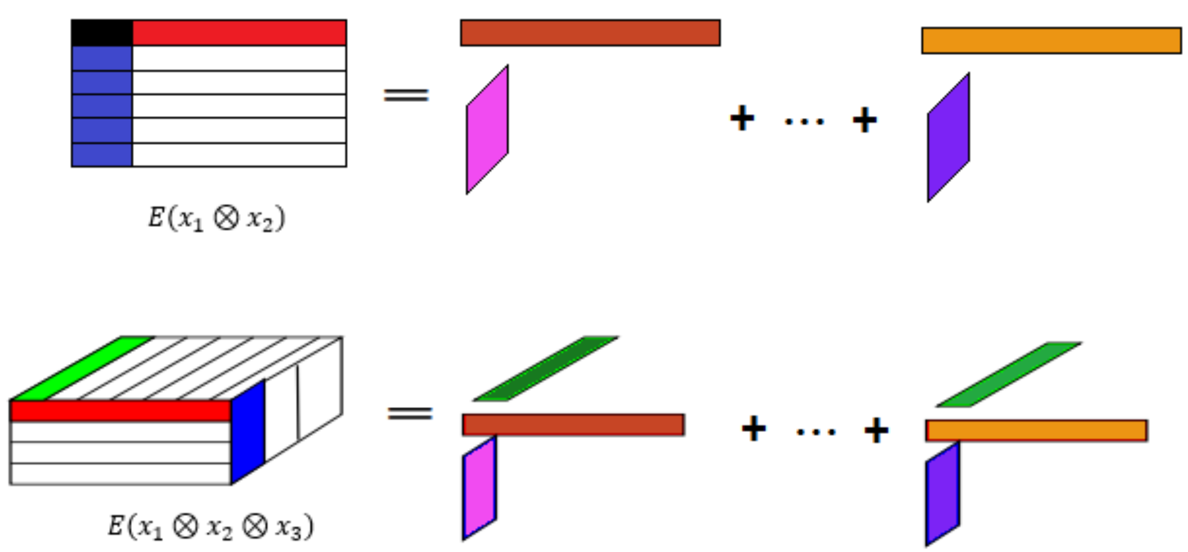


Method of Moment



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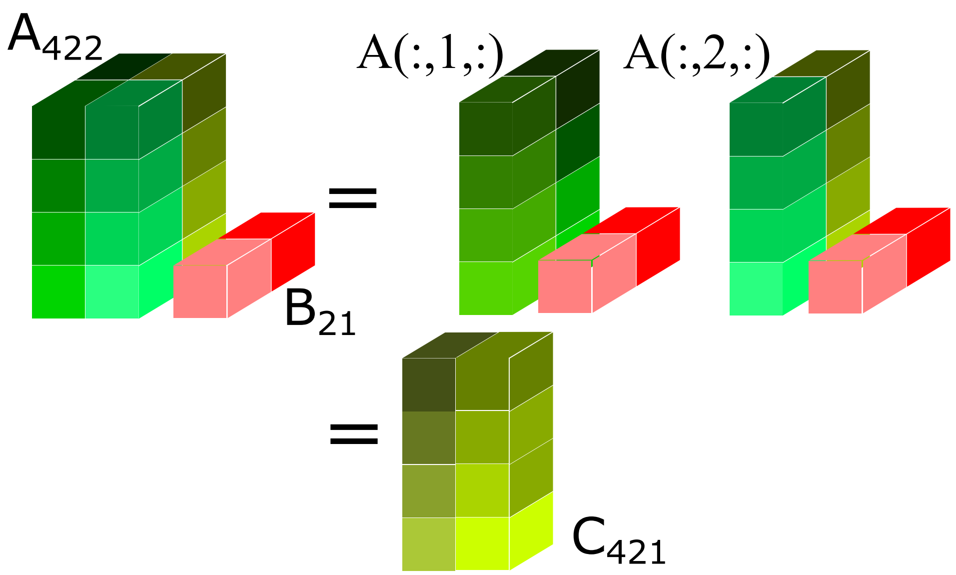
$$C_{\mathcal{C}} = A_{\mathcal{A}} \, B_{\mathcal{B}}$$



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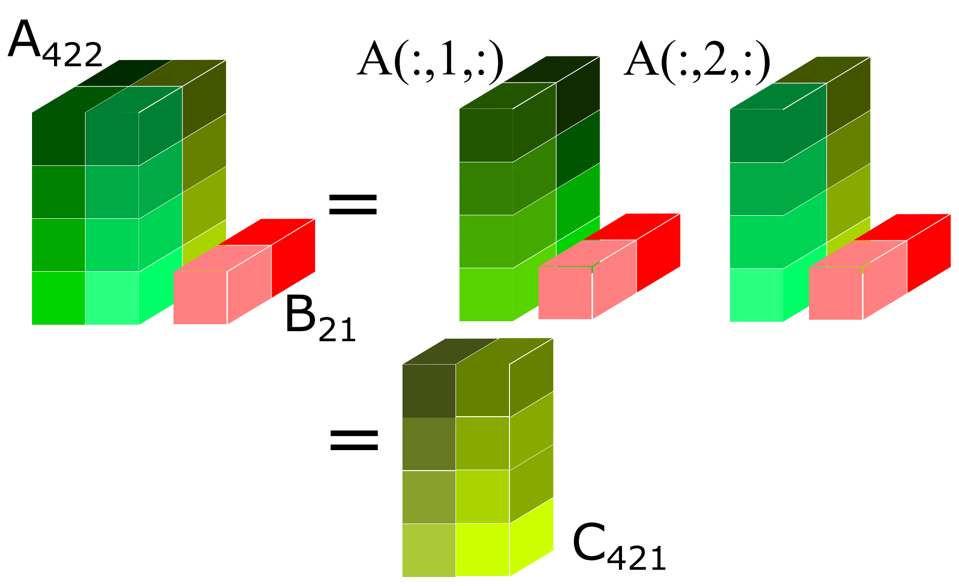

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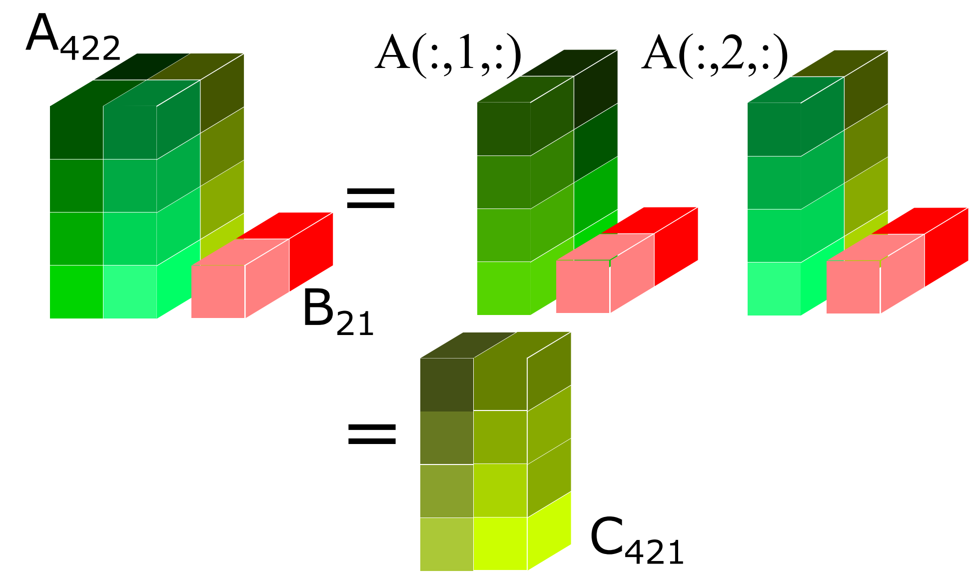
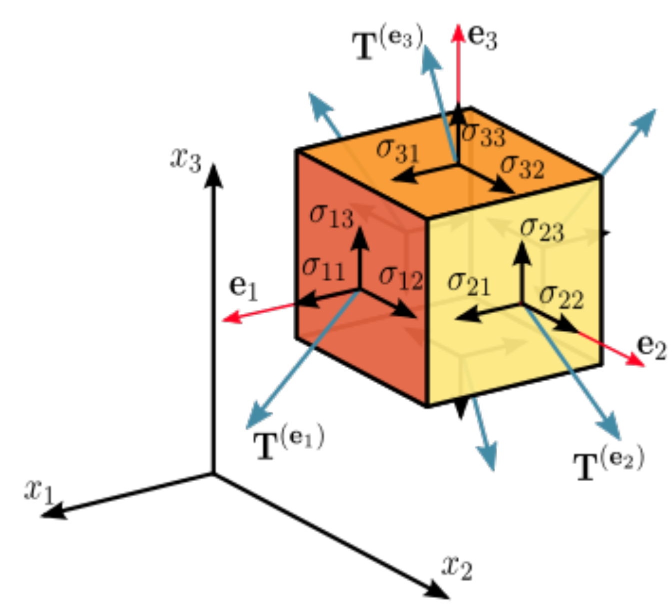


Why do we need tensor contraction?

- Physics
- Chemistry



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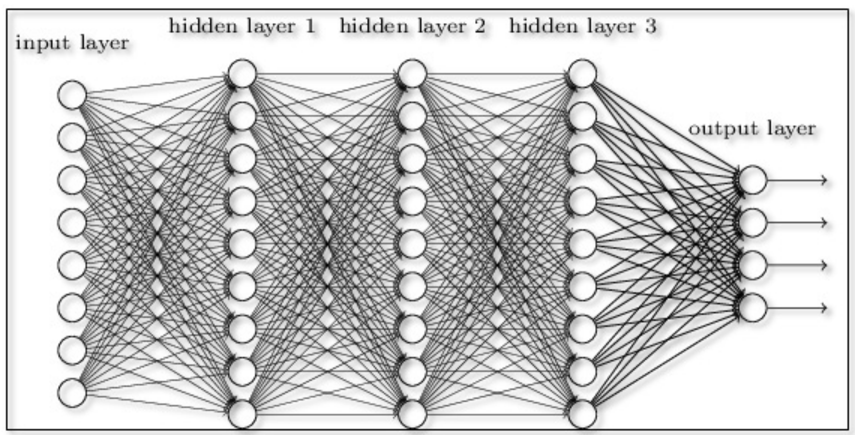

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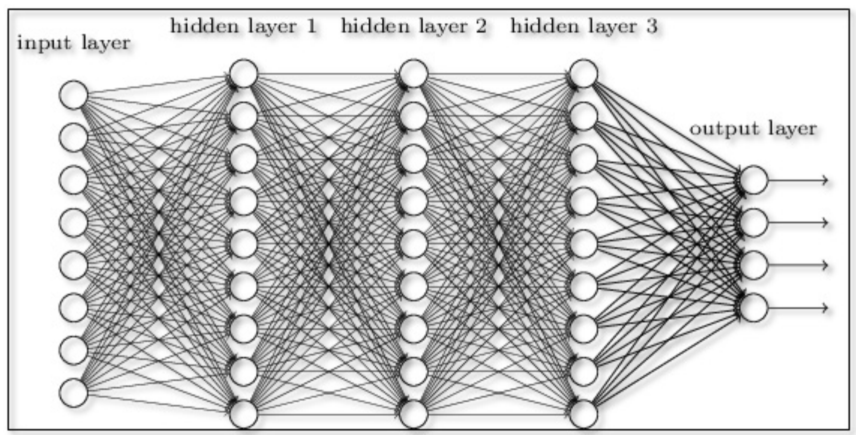

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  Example: Topic modeling

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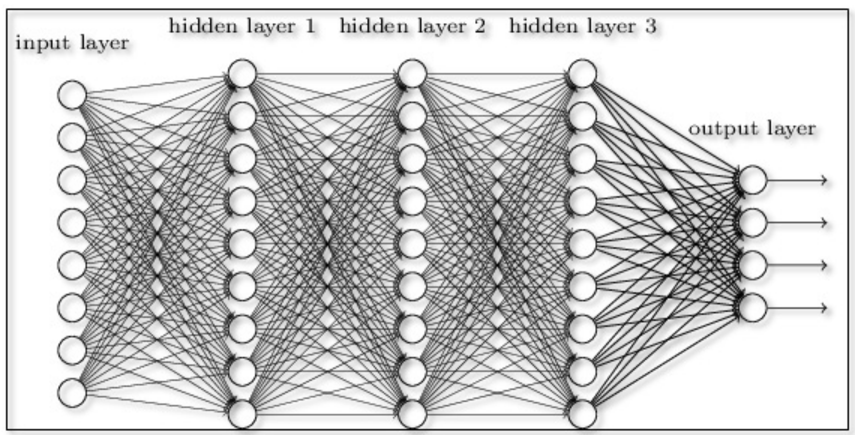

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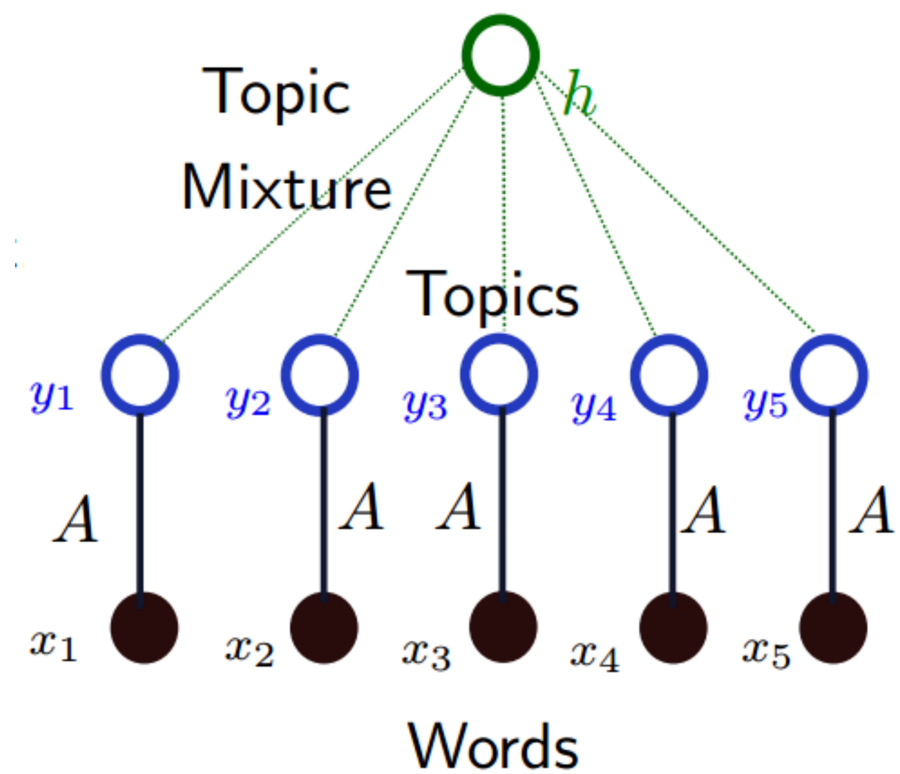

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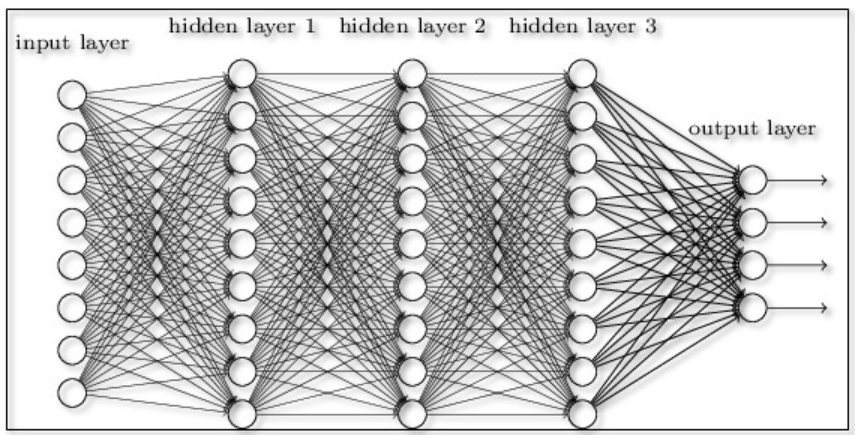

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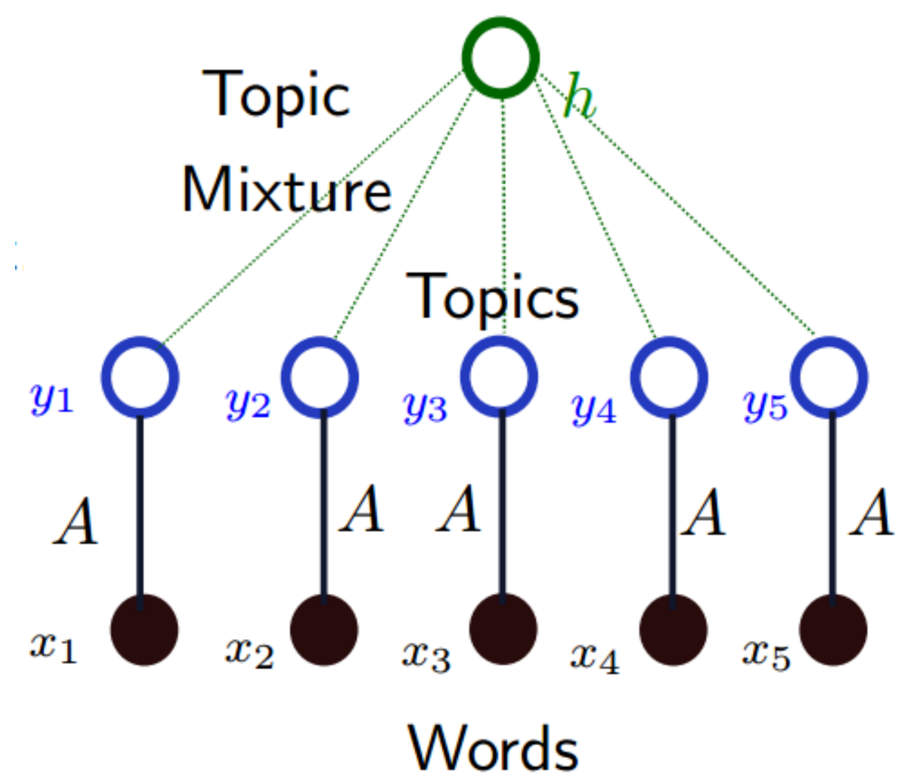
  h: Proportion of topics in a document

  $h = i$ with prob. w_i

  A: Topic-word matrix

  $$A(i,j) = \mathcal{P}(x_m = i | y_m = j)$$



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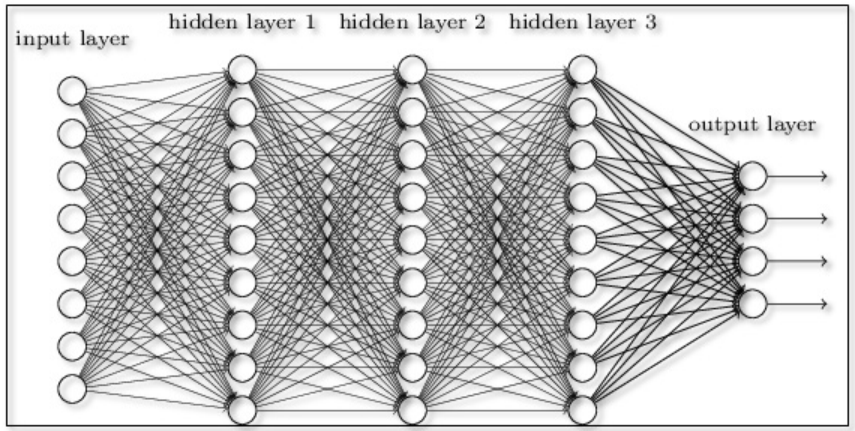

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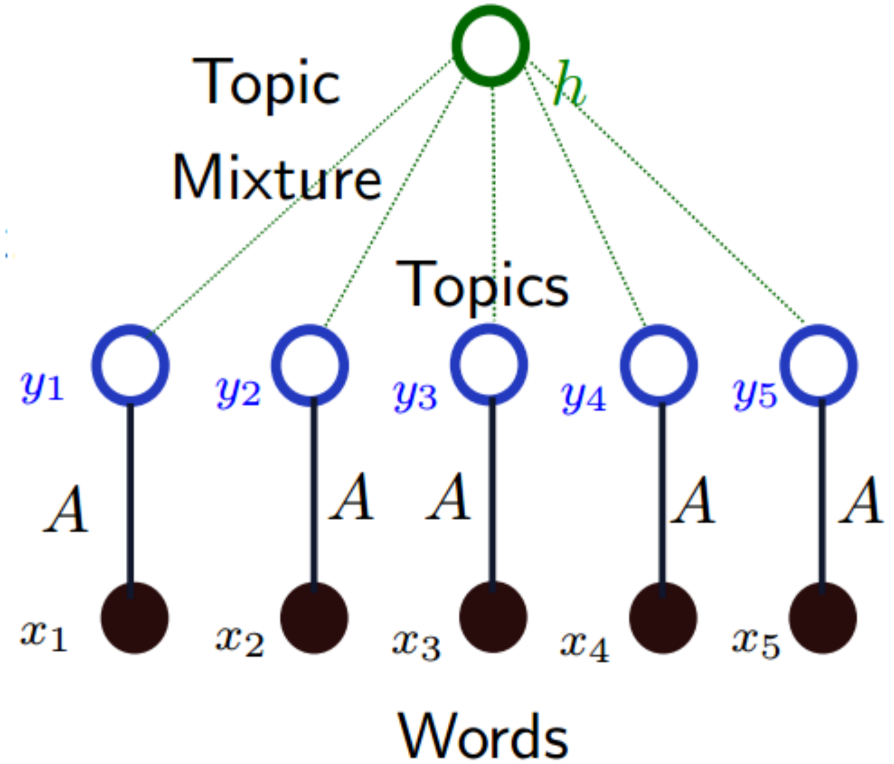
  Third order moment:

  $$M_3 = \mathbb{E}(x \otimes x \otimes x) = \sum_i w_i a_i \otimes a_i \otimes a_i$$



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- Parallel and distributed computing system: BatchedGEMM functions in MKL 11.3, CuBLAS v4.1: compute many matrix-matrix multiplies at once.

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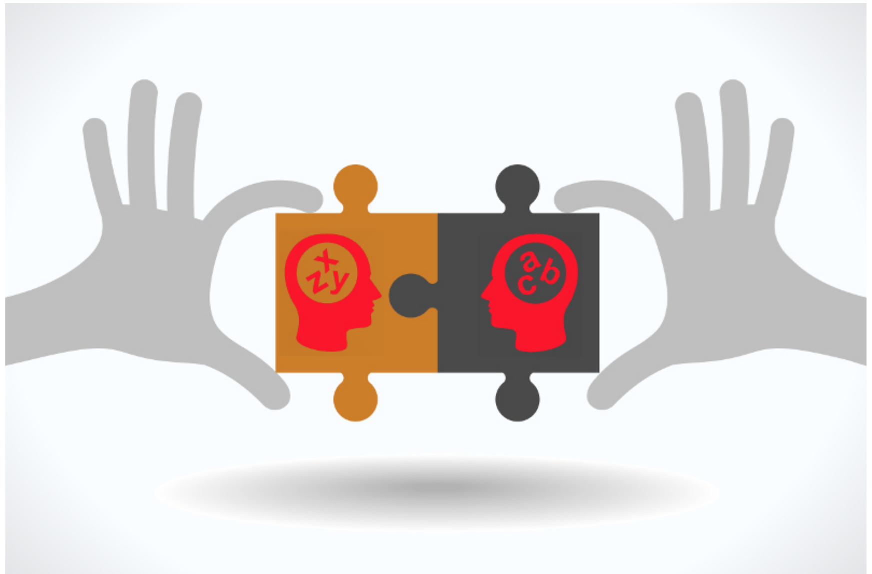

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$$A_{km} \rightarrow A_{mk}.$$
$$B_{pkn} \rightarrow B_{kpn}.$$
$$C_{mnp} \rightarrow C_{mpn}.$$
$$\boxed{C_{mpn} = A_{mk} B_{kpn}.}$$
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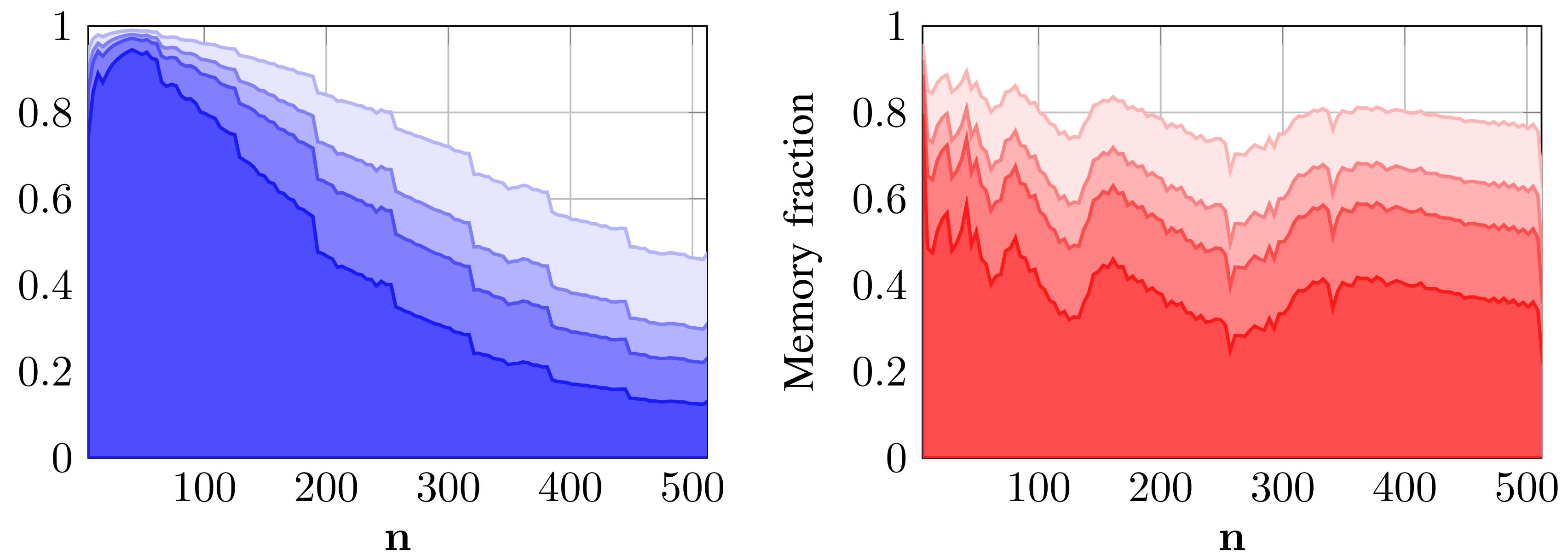

Figure: The fraction of time spent in copies/transpositions when computing Cmnp = AmkBpkn . Lines are shown with 1, 2, 3, and 6 total transpositions performed on either the input or output. (Left) CPU. (Right) GPU.

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- Introduce TensorLy: Tensor learning in python

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$y \leftarrow \alpha x + y$	$y \leftarrow \alpha op(A)x + \beta y$	$C \leftarrow \alpha op(A)op(B) + \beta C$

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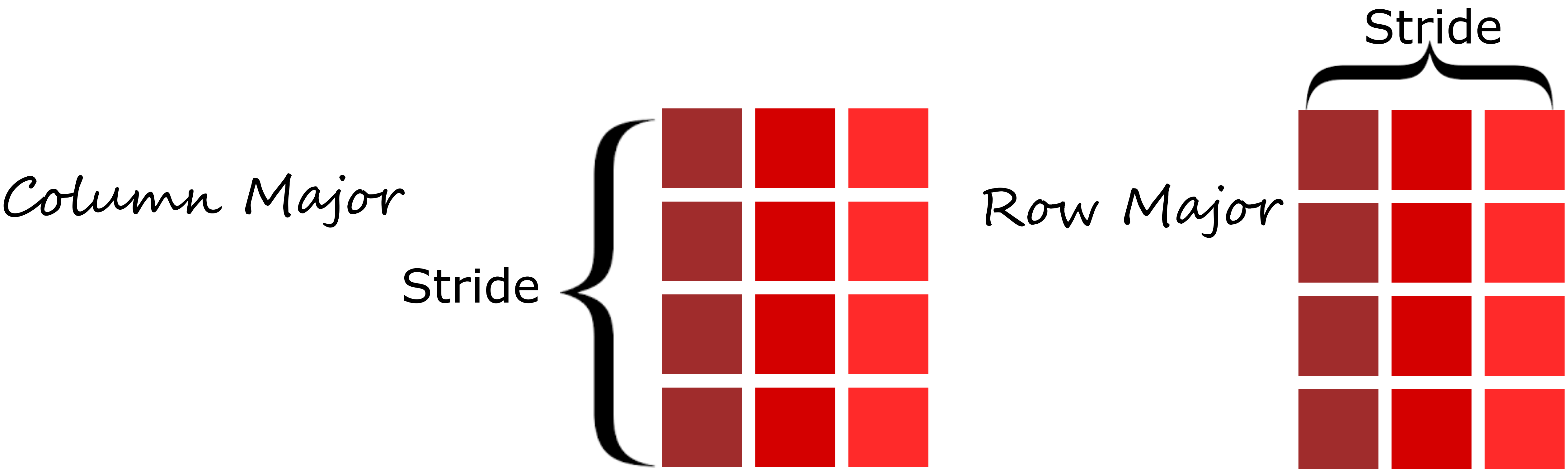

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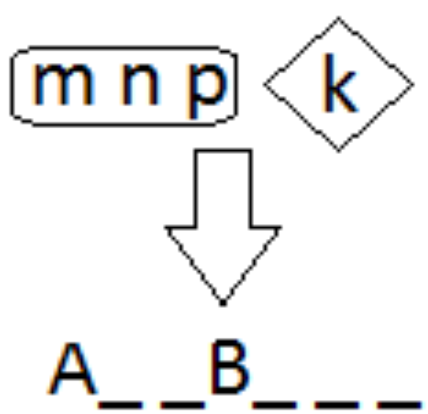
Focusing: one-index contraction

Extended BLAS Kernel for tensor one-index contraction

$$C = \alpha op(A) op(B) + \beta C$$

$$C_{mnp} = A_{**} \times B_{***}$$



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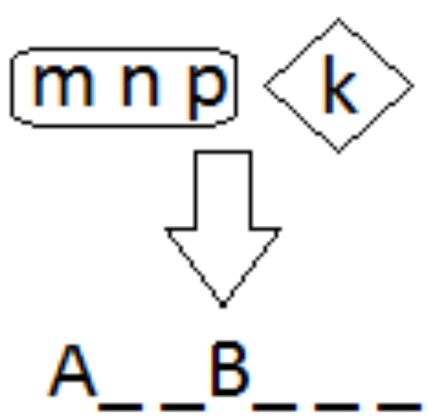

If fixing indices of C, there are total 3 x 2 x 3 x 2 x 1 = 36 cases.

Extended BLAS Operator

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Case	Contraction	Kernel1	Kernel2	Kernel3
1.1	$A_{mk}B_{knp}$	$C_{m(np)} = A_{mk}B_{k(np)}$	$C_{mn[p]} = A_{mk}B_{kn[p]}$	$C_{m[n]p} = A_{mk}B_{k[n]p}$

Table: Example: possible mappings to Level 3 BLAS routines

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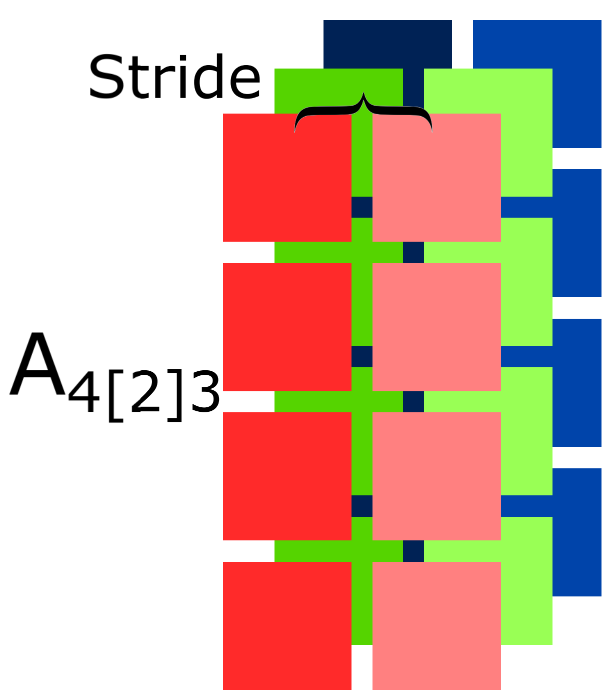

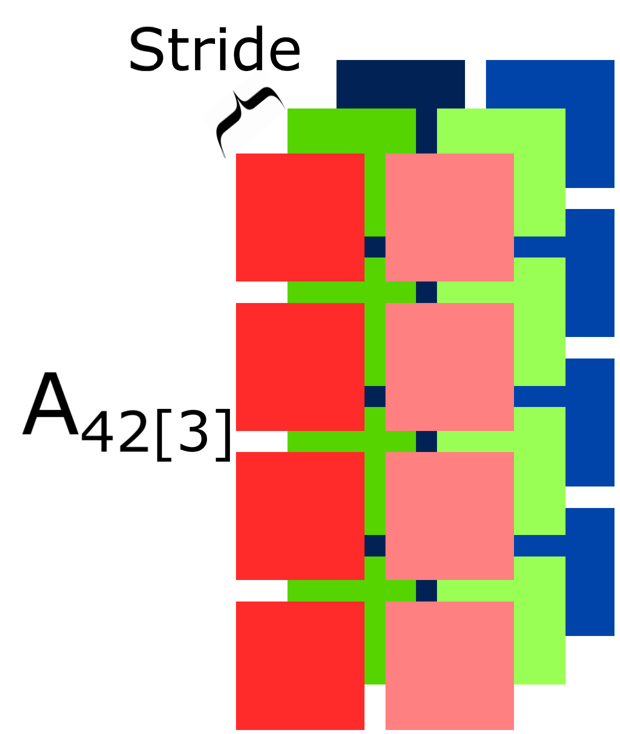

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1.2	$A_{mk}B_{kpn}$	$C_{mn[p]} = A_{mk}B_{k[p]n}$	$C_{m[n]p} = A_{mk}B_{kp[n]}$	
1.3	$A_{mk}B_{nkp}$	$C_{mn[p]} = A_{mk}B^\top_{nk[p]}$		
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1.5	$A_{mk}B_{npk}$	$C_{m(np)} = A_{mk}B^\top_{(np)k}$	$C_{mn[p]} = A_{mk}B^\top_{n[p]k}$	
1.6	$A_{mk}B_{pnk}$	$C_{m[n]p} = A_{mk}B^\top_{p[n]k}$		
2.1	$A_{km}B_{knp}$	$C_{m(np)} = A^\top_{km}B_{k(np)}$	$C_{mn[p]} = A^\top_{km}B_{kn[p]}$	$C_{m[n]p} = A^\top_{km}B_{k[n]p}$
2.2	$A_{km}B_{kpn}$	$C_{mn[p]} = A^\top_{km}B_{k[p]n}$	$C_{m[n]p} = A^\top_{km}B_{kp[n]}$	
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3.1	$A_{nk}B_{kmp}$	$C_{mn[p]} = B^\top_{km[p]}A^\top_{nk}$		
3.2	$A_{nk}B_{kpm}$	$C_{mn[p]} = B^\top_{k[p]m}A^\top_{nk}$		
3.3	$A_{nk}B_{mkp}$	$C_{mn[p]} = B_{mk[p]}A^\top_{nk}$		
3.4	$A_{nk}B_{pkm}$	$TRANS(A_{nk}B^\top_{pk[m]})$	$C_{[m][n]p} = B_{pk[m]}A_{[n]k}$	
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Case	Contraction	Kernel1	Kernel2
4.1	$A_{kn}B_{kmp}$	$C_{mn[p]} = B^\top_{km[p]}A_{kn}$	
4.2	$A_{kn}B_{kpm}$	$C_{mn[p]} = B^\top_{k[p]m}A_{kn}$	
4.3	$A_{kn}B_{mkp}$	$C_{mn[p]} = B_{mk[p]}A_{kn}$	
4.4	$A_{kn}B_{pkm}$	$TRANS(A^\top_{kn}B^\top_{pk[m]})$	$C_{[m][n]p} = B_{pk[m]}A_{k[n]}$
4.5	$A_{kn}B_{mpk}$	$C_{mn[p]} = B_{m[p]k}A_{kn}$	
4.6	$A_{kn}B_{pmk}$	$TRANS(A^\top_{kn}B^\top_{p[m]k})$	$C_{[m][n]p} = B_{p[m]k}A_{k[n]}$
5.1	$A_{pk}B_{kmn}$	$C_{(mn)p} = B^\top_{k(mn)}A^\top_{pk}$	$C_{m[n]p} = B^\top_{km[n]}A^\top_{pk}$
5.2	$A_{pk}B_{knm}$	$C_{m[n]p} = B^\top_{k[n]m}A^\top_{pk}$	
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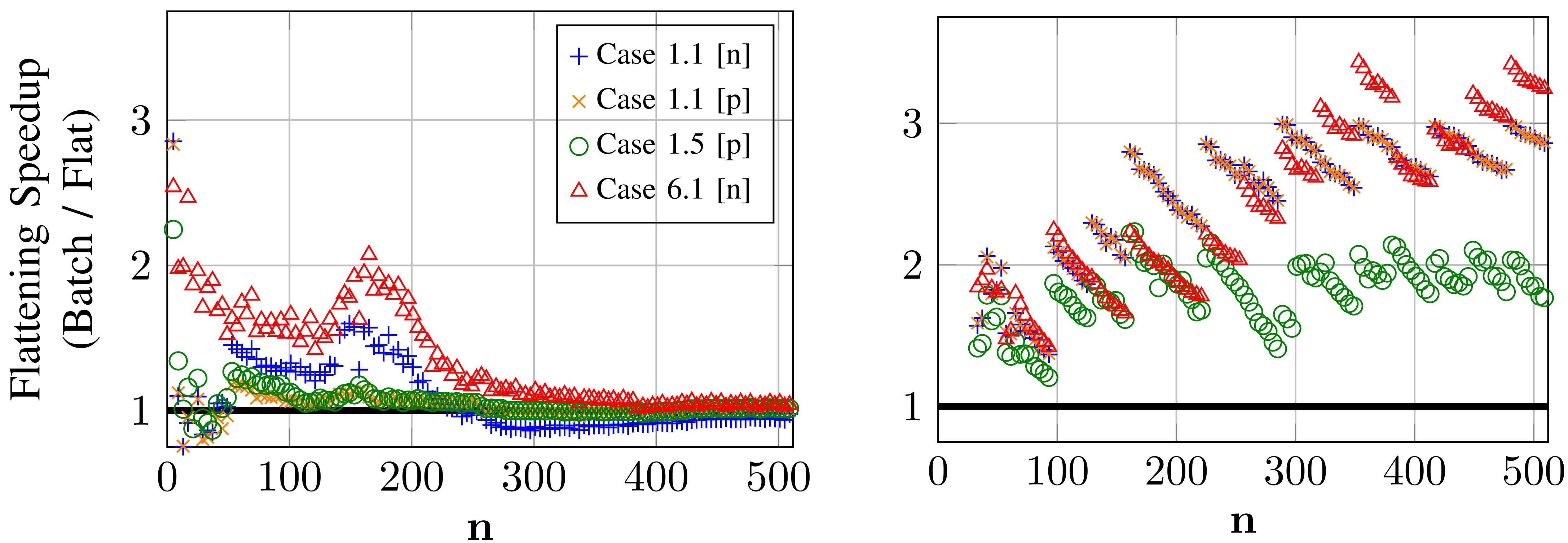
2.3	$A_{km}B_{nkp}$	$C_{mn[p]} = A^{\top}_{km}B^{\top}_{nk[p]}$			5.3	$A_{pk}B_{mkn}$	$C_{m[n]p} = B_{mk[n]}A^{\top}_{pk}$	
2.4	$A_{km}B_{pkn}$	$C_{m[n]p} = A^{\top}_{km}B^{\top}_{pk[n]}$			5.4	$A_{pk}B_{nkm}$	$TRANS(B_{nk[m]}A^{\top}_{pk})$	$C_{[m]n[p]} = B_{nk[m]}A_{[p]k}$
2.5	$A_{km}B_{npk}$	$C_{m(np)} = A^{\top}_{km}B^{\top}_{(np)k}$	$C_{mn[p]} = A^{\top}_{km}B^{\top}_{n[p]k}$		5.5	$A_{pk}B_{mnk}$	$C_{(mn)p} = B_{(mn)k}A^{\top}_{pk}$	$C_{m[n]p} = B_{m[n]k}A^{\top}_{pk}$
2.6	$A_{km}B_{pnk}$	$C_{m[n]p} = A^{\top}_{km}B^{\top}_{p[n]k}$			5.6	$A_{pk}B_{nmk}$	$TRANS(B_{n[m]k}A^{\top}_{pk})$	$C_{[m]n[p]} = B_{n[m]k}A_{[p]k}$
3.1	$A_{nk}B_{kmp}$	$C_{mn[p]} = B^{\top}_{km[p]}A^{\top}_{nk}$			6.1	$A_{kp}B_{kmn}$	$C_{(mn)p} = B^{\top}_{k(mn)}A_{kp}$	$C_{m[n]p} = B^{\top}_{km[n]}A_{kp}$
3.2	$A_{nk}B_{kpm}$	$C_{mn[p]} = B^{\top}_{k[p]m}A^{\top}_{nk}$			6.2	$A_{kp}B_{knm}$	$C_{m[n]p} = B^{\top}_{k[n]m}A_{kp}$	
3.3	$A_{nk}B_{mkp}$	$C_{mn[p]} = B_{mk[p]}A^{\top}_{nk}$			6.3	$A_{kp}B_{mkn}$	$C_{m[n]p} = B_{mk[n]}A_{kp}$	
3.4	$A_{nk}B_{pkm}$	$TRANS(A_{nk}B^{\top}_{pk[m]})$	$C_{[m][n]p} = B_{pk[m]}A_{[n]k}$		6.4	$A_{kp}B_{nkm}$	$TRANS(B_{nk[m]}A_{kp})$	$C_{[m]n[p]} = B_{nk[m]}A_{k[p]}$
3.5	$A_{nk}B_{mpk}$	$C_{mn[p]} = B_{m[p]k}A^{\top}_{nk}$			6.5	$A_{kp}B_{mnk}$	$C_{(mn)p} = B_{(mn)k}A_{kp}$	$C_{m[n]p} = B_{m[n]k}A_{kp}$
3.6	$A_{nk}B_{pmk}$	$TRANS(A_{nk}B^{\top}_{p[m]k})$	$C_{[m][n]p} = B_{p[m]k}A_{[n]k}$		6.6	$A_{kp}B_{nmk}$	$TRANS(B_{n[m]k}A_{kp})$	$C_{[m]n[p]} = B_{n[m]k}A_{k[p]}$

Table: List of 36 possible single mode contraction operations between a second-order tensor and a third-order tensor and possible mappings to Level-3 BLAS routines

Analysis

Flatten v.s. SBGEMM

Case	Contraction	Kernel1	Kernel2	Kernel3
1.1	$A_{mk}B_{knp}$	$C_{m(np)} = A_{mk}B_{k(np)}$	$C_{mn[p]} = A_{mk}B_{kn[p]}$	$C_{m[n]p} = A_{mk}B_{k[n]p}$

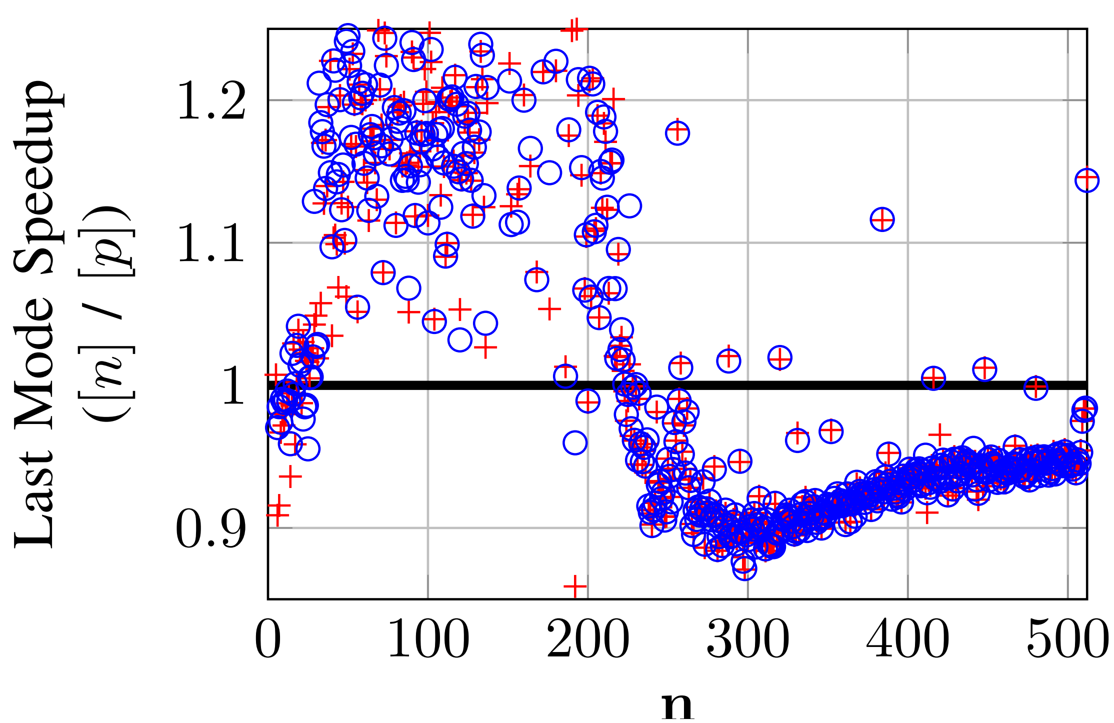


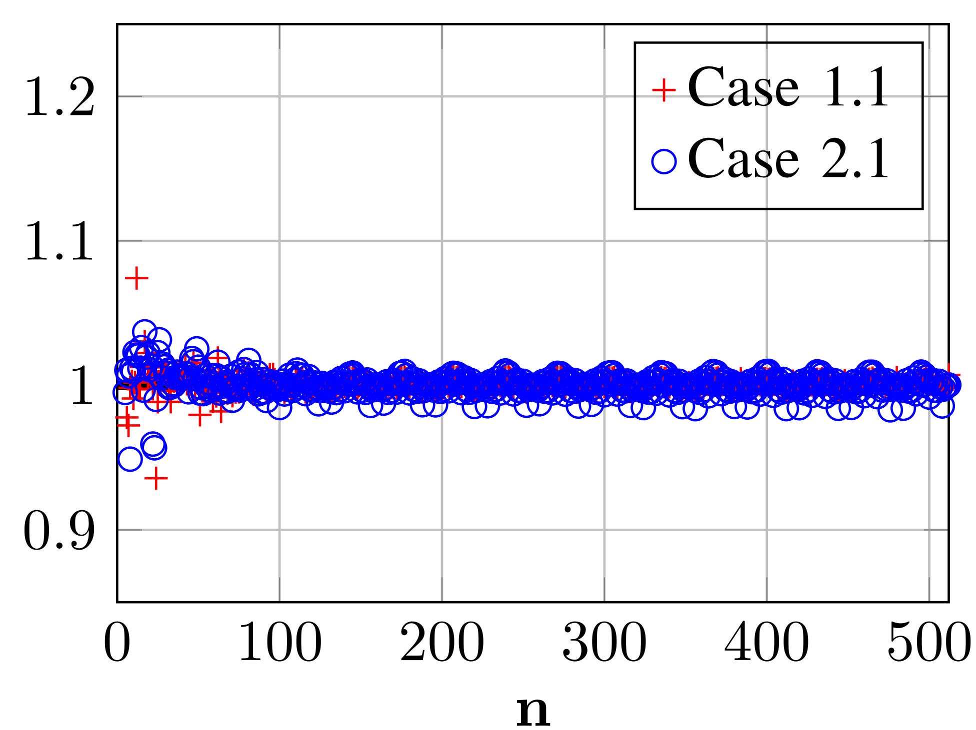
Prefer flatten than SBGEMM

Analysis

Batching in last mode v.s. middle mode

Case	Contraction	Kernel1	Kernel2	Kernel3
1.1	$A_{mk}B_{knp}$	$C_{m(np)} = A_{mk}B_{k(np)}$	$C_{mn[p]} = A_{mk}B_{kn[p]}$	$C_{m[n]p} = A_{mk}B_{k[n]p}$
2.1	$A_{km}B_{knp}$	$C_{m(np)} = A_{km}^\top B_{k(np)}$	$C_{mn[p]} = A_{km}^\top B_{kn[p]}$	$C_{m[n]p} = A_{km}^\top B_{k[n]p}$





On CPU, it’s better to batch in last mode when tensor size is small/moderate

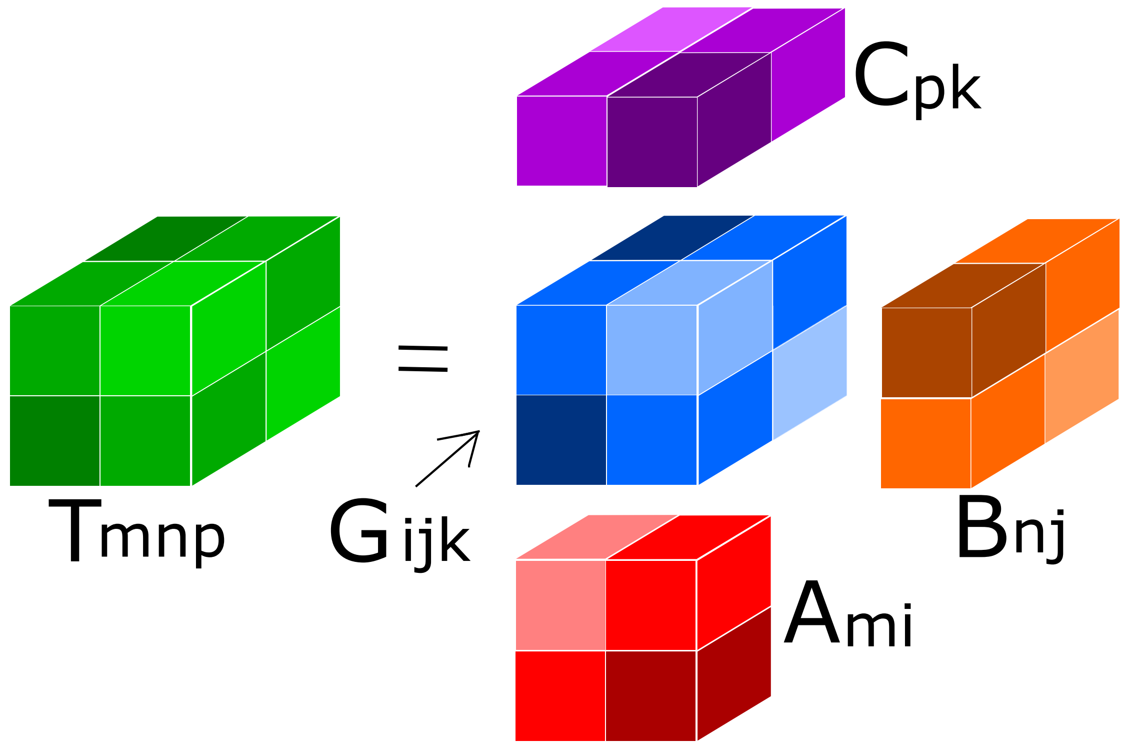
Application: Tucker Decomposition

Application: Tucker Decomposition

$$T_{mnp} = G_{ijk} A_{mi} B_{nj} C_{pk}$$

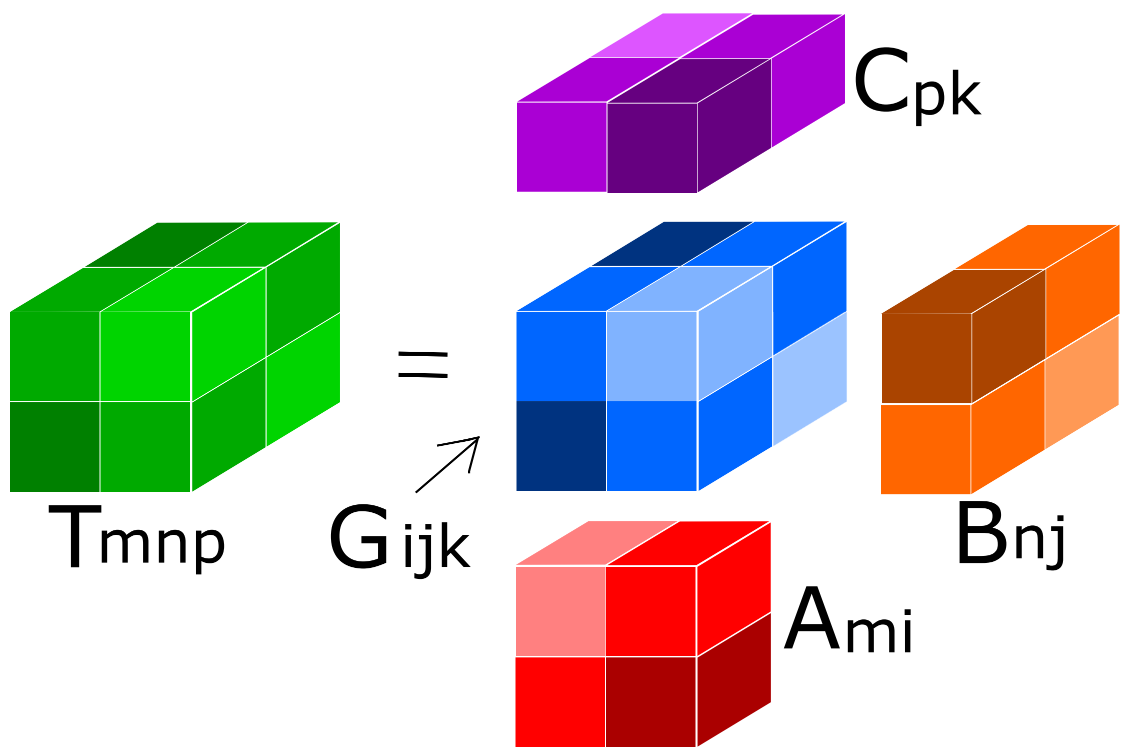
Application: Tucker Decomposition

$$T_{mnp} = G_{ijk} A_{mi} B_{nj} C_{pk}$$



Application: Tucker Decomposition

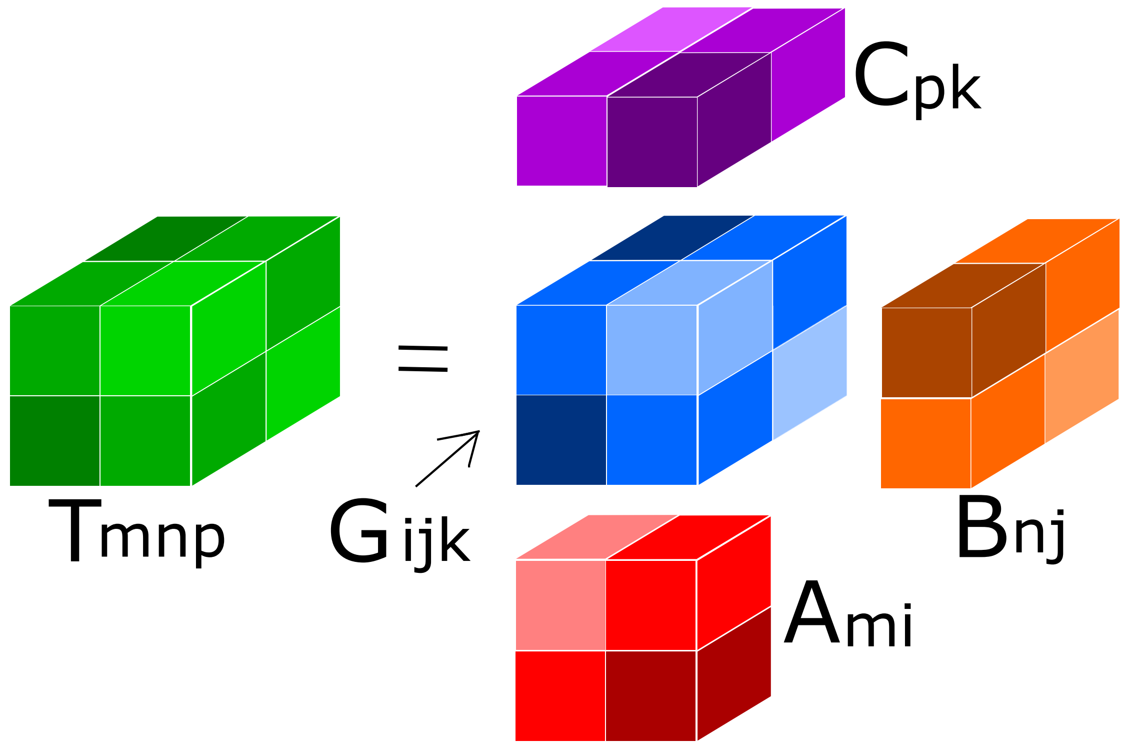
$$T_{mnp} = G_{ijk} A_{mi} B_{nj} C_{pk}$$



Main Steps:

Application: Tucker Decomposition

$$T_{mnp} = G_{ijk} A_{mi} B_{nj} C_{pk}$$



Main Steps:

- $Y_{mjk} = T_{mnp} B^t_{nj} C^t_{pk}$
- $Y_{ink} = T_{mnp} A^{t+1}_{mi} C^t_{pk}$
- $Y_{ijp} = T_{mnp} B^{t+1}_{nj} A^{t+1}_{mi}$

Application: Tucker Decomposition

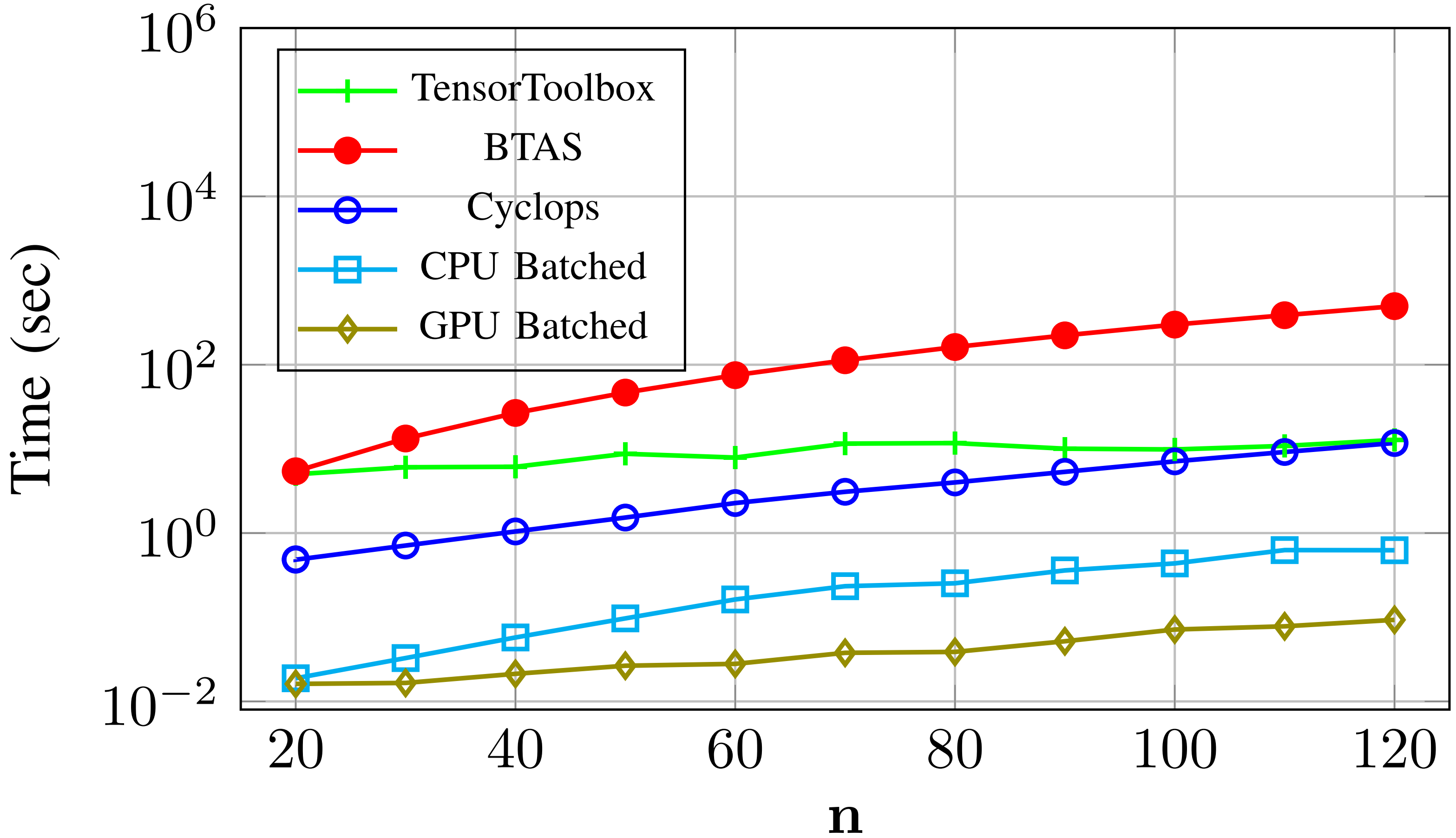


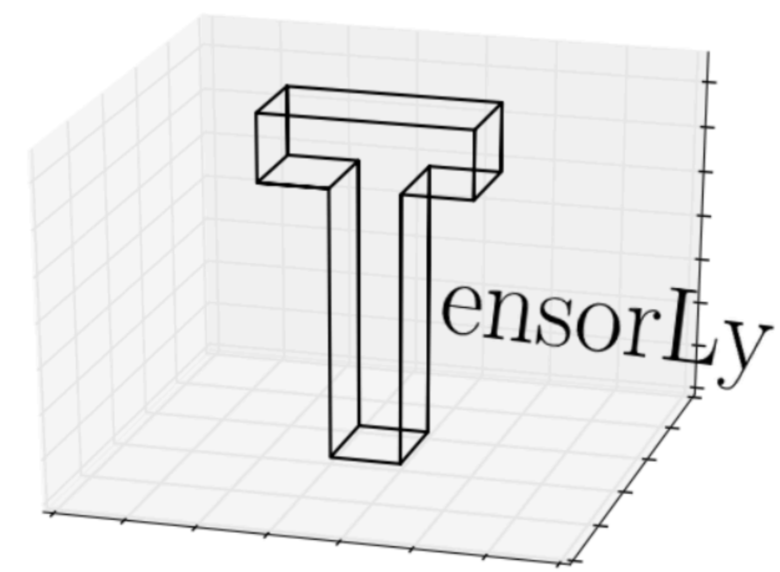
Figure: Performance on Tucker decomposition.

Conclusion

- StridedBatchedGEMM for generalized tensor contractions.
- Avoid explicit transpositions or permutations.
- 10x(GPU) and 2x(CPU) speedup on small and moderate sized tensors.
- Available in CuBLAS 8.0.

Introduction of TensorLy

by Jean Kossaifi, Imperial College London
Yannis Panagakis, Imperial College London
Anima Anandkumar, Caltech



Introduction of TensorLy

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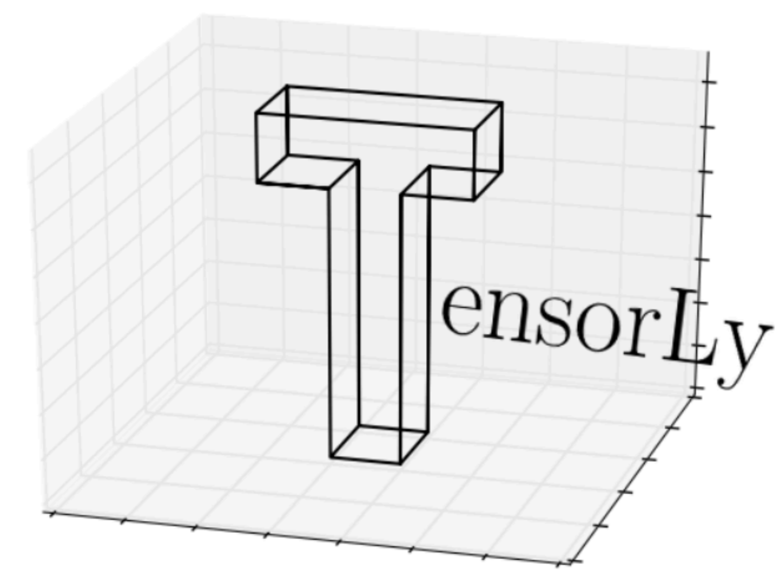
- **Open source**

Homepage: http://tensorly.org/dev/

Github: https://github.com/tensorly/tensorly

Suitable for academic / industrial applications



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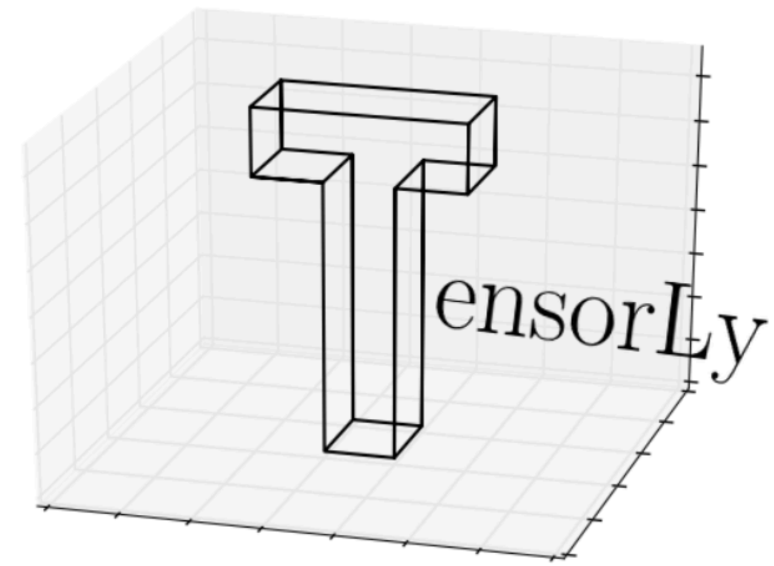


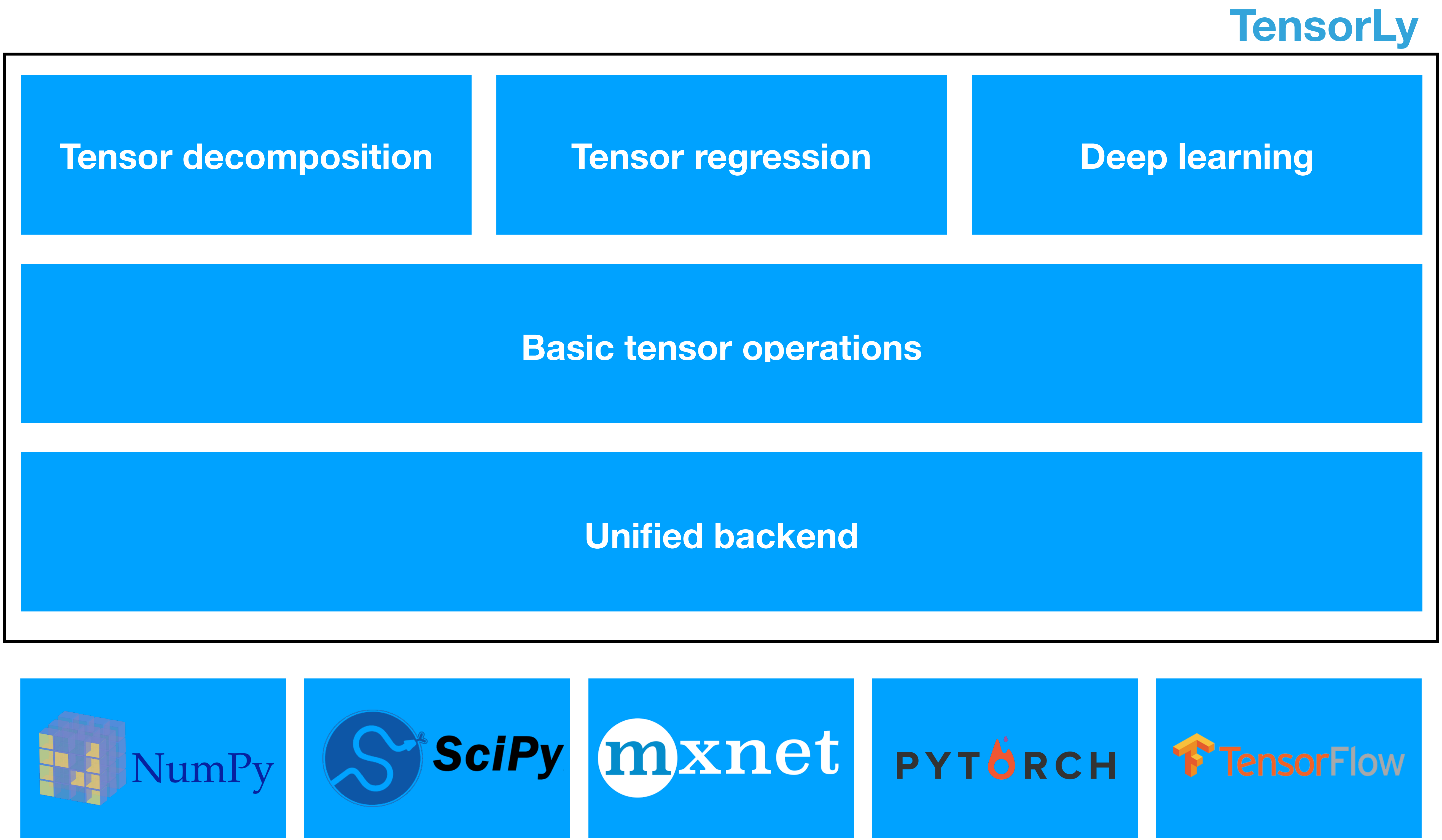
- **Reliability and easy to use**

  Depends only on NumPy, SciPy [Optionally Matplotlib, MXNet and PyTorch]

  Exhaustive documentation, Unit-testing for all functions

  Fast

User-friendly API



TensorLy Operators

- Kronecker
- Khatri-rao
- Hadamard products
- Tensor unfolding/folding/vectorization
- N-mode product

`khatri_rao` (matrices[, skip_matrix, reverse])	Khatri-Rao product of a list of matrices
`kronecker` (matrices[, skip_matrix, reverse])	Kronecker product of a list of matrices
`mode_dot` (tensor, matrix_or_vector, mode)	n-mode product of a tensor and a matrix or vector at the specified mode
`multi_mode_dot` (tensor, matrix_or_vec_list[, …])	n-mode product of a tensor and several matrices or vectors over several modes
`proximal.soft_thresholding` (tensor, threshold)	Soft-thresholding operator
`proximal.svd_thresholding` (matrix, threshold)	Singular value thresholding operator
`proximal.procrustes` (matrix)	Procrustes operator
`inner` (tensor1, tensor2[, n_modes])	Generalised inner products between tensors

- CANONICAL-POLYADIC (CP)
- Non-negative CP Tucker (HO-SVD)
- Non-negative Tucker
- Robust Tensor PCA

`parafac` (tensor, rank[, n_iter_max, init, …])	CANDECOMP/PARAFAC decomposition via alternating least squares (ALS)
`non_negative_parafac` (tensor, rank[, …])	Non-negative CP decomposition
`tucker` (tensor[, rank, ranks, n_iter_max, …])	Tucker decomposition via Higher Order Orthogonal Iteration (HOI)
`partial_tucker` (tensor, modes[, rank, …])	Partial tucker decomposition via Higher Order Orthogonal Iteration (HOI)
`non_negative_tucker` (tensor, rank[, …])	Non-negative Tucker decomposition
`robust_pca` (X[, mask, tol, reg_E, reg_J, …])	Robust Tensor PCA via ALM with support for missing values

TensorLy Example

```python
from tensorly.decomposition import parafac

factors = parafac(image, rank=50, init='random')
cp_reconstruction = tl.kruskal_to_tensor(factors)
```

```python
from tensorly.decomposition import tucker

core, factors = tucker(image, ranks=(50, 50, 3), init='random')
tucker_reconstruction = tl.tucker_to_tensor(core, factors)
```

original

CP

Tucker

TensorLy Backend

tl.set_backend(‘numpy’) # or ‘mxnet’ or ‘pytorch’

```
import tensorly as tl

T = tl.tensor([[1, 2, 3], [4, 5, 6]])
tl.tenalg.kronecker([T, T])
tl.clip(T, a_min=2, a_max=5)

tl.set_backend('mxnet')
T = tl.tensor([[1, 2, 3], [4, 5, 6]])

tl.set_backend('pytorch')
T = tl.tensor([[1, 2, 3], [4, 5, 6]])
```

NumPy ndarray

MXNet NDArray

PyTorch FloatTensor

TensorLy Example

Back-propagate through tensor operations with PyTorch

```
import tensorly as tl
from tensorly.random import tucker_tensor

tl.set_backend('pytorch')
core, factors = tucker_tensor((5, 5, 5),
                              rank=(3, 3, 3))
core = Variable(core, requires_grad=True)
factors = [Variable(f, requires_grad=True) for f in factors]

optimiser = torch.optim.Adam([core]+factors, lr=lr)

for i in range(1, n_iter):
    optimiser.zero_grad()
    rec = tucker_to_tensor(core, factors)
    loss = (rec - tensor).pow(2).sum()
    for f in factors:
        loss = loss + 0.01*f.pow(2).sum()

    loss.backward()
    optimiser.step()
```

PyTorch FloatTensor

We can attach gradients

Penalty on the factors

Contribute to TensorLy

Contributions welcome!

- If you have a cool tensor method you want to add
- If you spot a bug

Thank you!

Questions?