Batched algorithm for tensor contraction in Ambit

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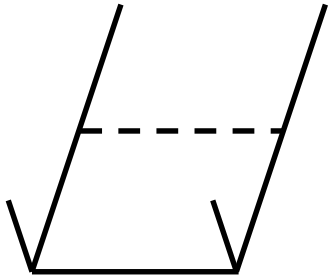
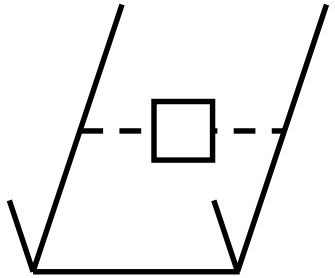
Density fitting saves memory… Oops!



v^4

$$R_{ij}^{ef} \mathrel{+}= t_{ij}^{ab}\langle ab|ef\rangle$$

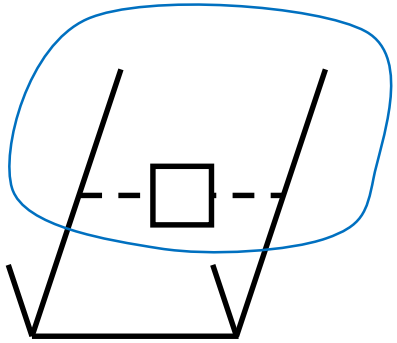


$v^2 L$

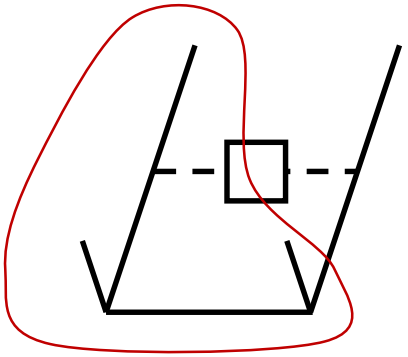
$o^2 v^2$

?

$$R_{ij}^{ef} \mathrel{+}= t_{ij}^{ab} B_{ae}^{L} B_{bf}^{L}$$



v^4

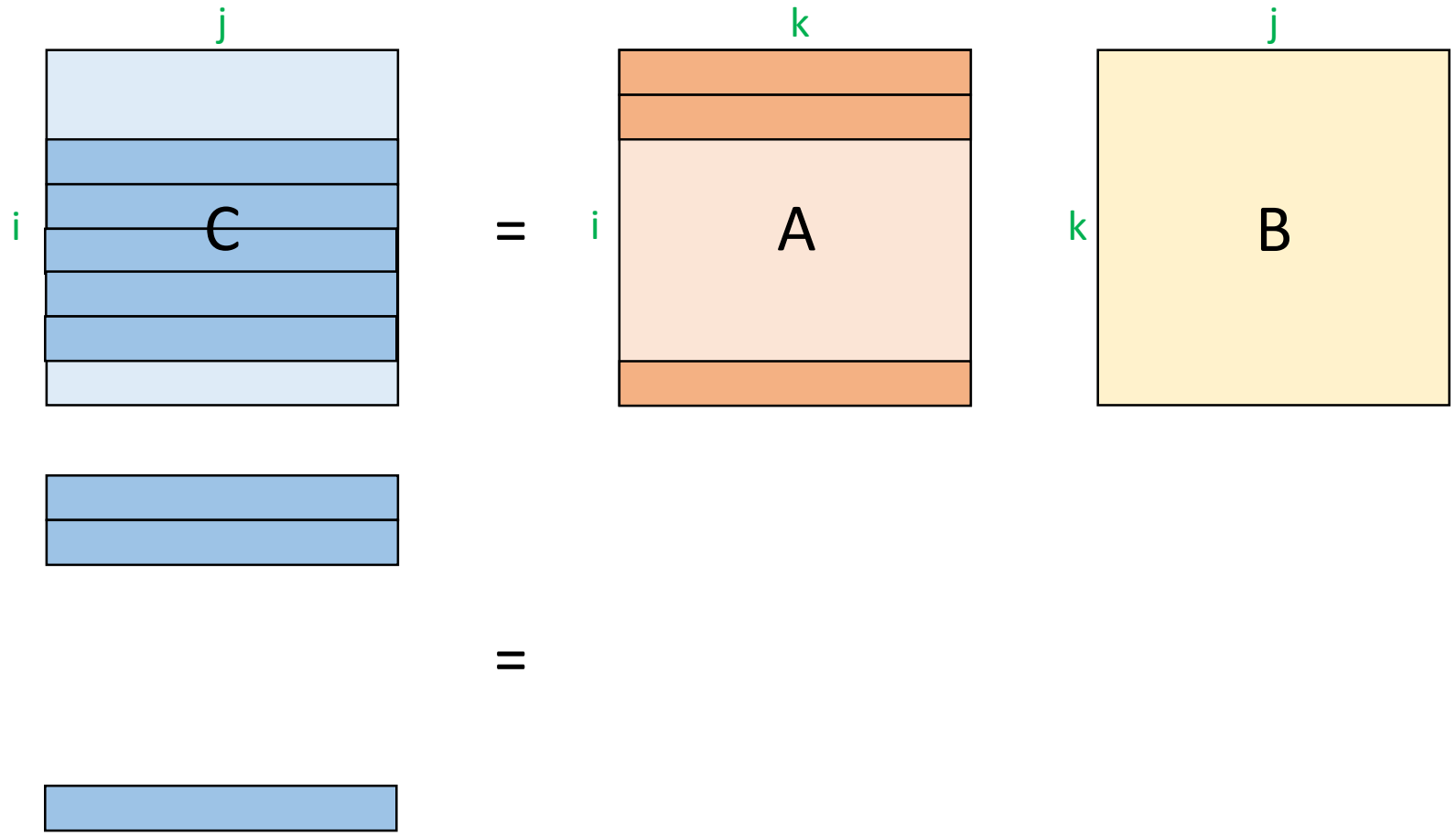


$o^2 v^2 L$

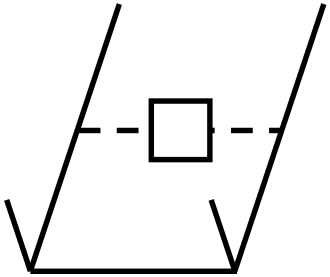
- $V_{aebf} = B_{ae}^{L} B_{bf}^{L}$
- $R_{ij}^{ef} \mathrel{+}= t_{ij}^{ab} V_{aebf}$

- $I_{ije}^{bL} = t_{ij}^{ab} B_{ae}^{L}$
- $R_{ij}^{ef} \mathrel{+}= I_{ije}^{bL} B_{bf}^{L}$

- $C_j^i = A_k^i B_j^k$
- C[“ij”] = A[“ik”] * B[“kj”];

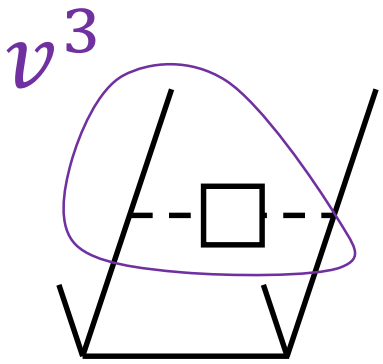


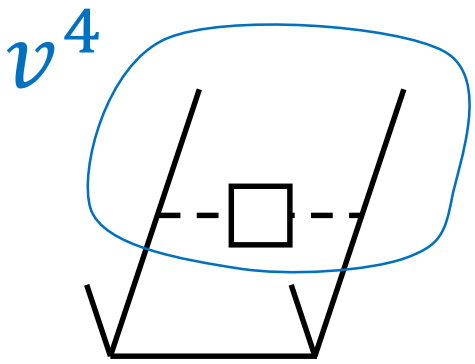
- $R_{ij}^{ef} \mathrel{+}= t_{ij}^{ab} B_{ae}^{L} B_{bf}^{L}$
- R[“efij”] += T[“abij”] * B[“Lae”] * B[“Lbf”];



V[“aebf”]

- Loop over f:
  - $B_{b[f]}^{L} \rightarrow B'^{L}_{b}$
  - $V'_{aeb} = B_{ae}^{L} B'^{L}_{b}$
  - $R'^{e}_{ij} \mathrel{+}= t_{ij}^{ab} V'_{aeb}$
  - $R_{ij}^{e[f]} \leftarrow R'^{e}_{ij}$





- R[“efij”] += T[“abij”] * B[“Lae”] * B[“Lbf”];

R’’[“feij”] B’’[“fLb”] Permuted stage

R’[“eij”] V’[“aeb”] B’[“Lb”] Batched stage

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Thank you!