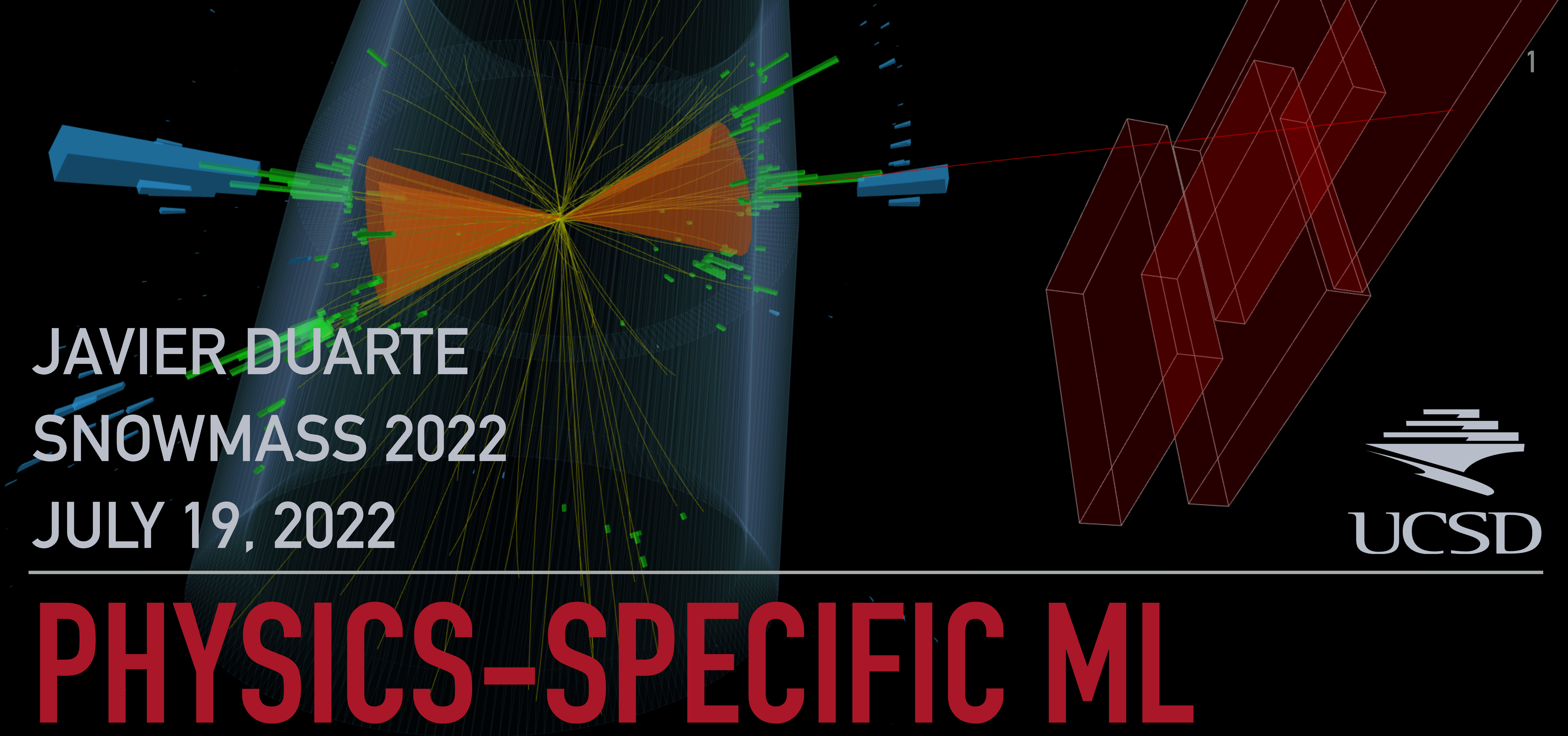


JAVIER DUARTE

SNOWMASS 2022

JULY 19, 2022

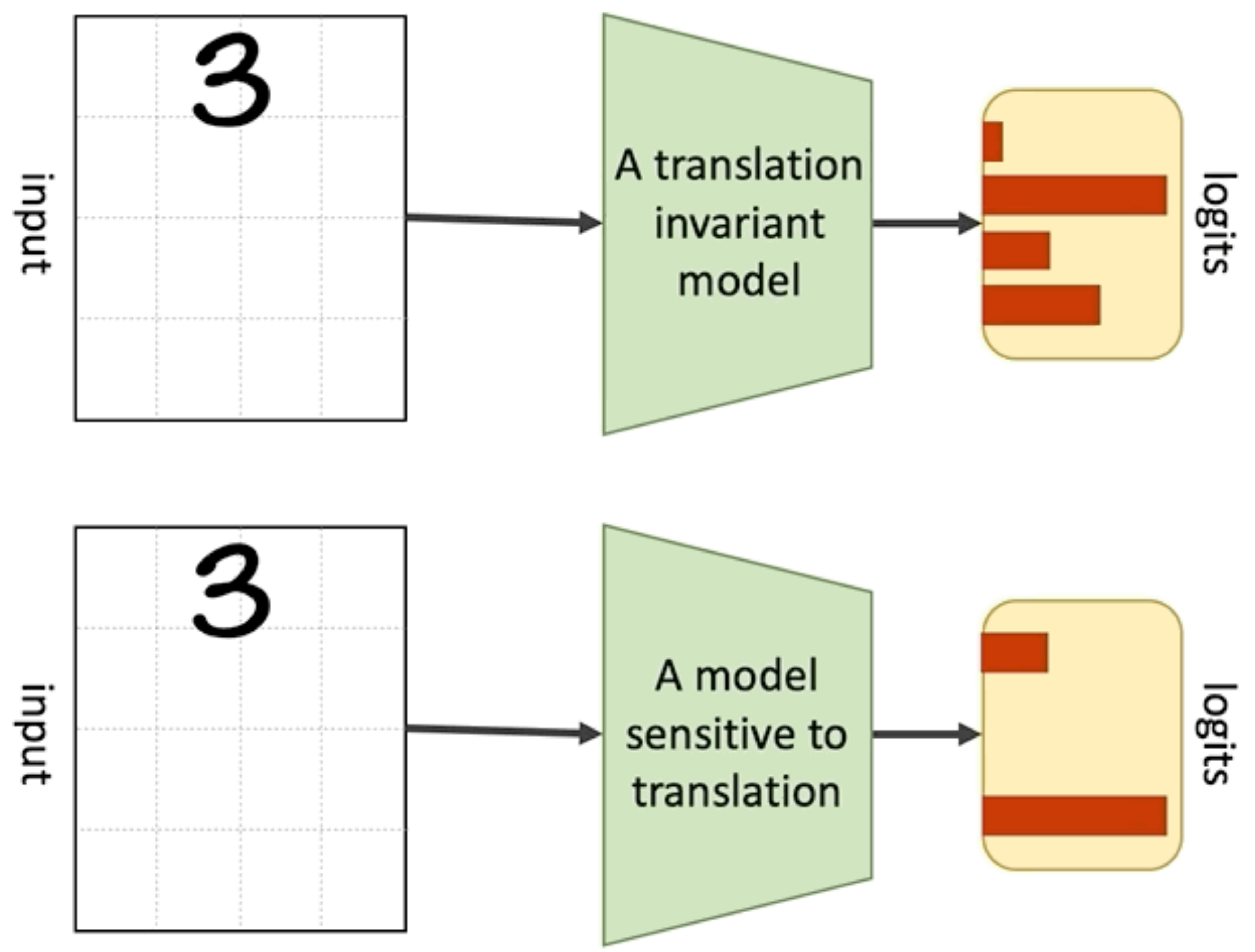
UCSD

PHYSICS-SPECIFIC ML FOR DATA ANALYSIS

SCOPE: INDUCTIVE BIAS

dropbox.com/s/o3ehw70ou6rpsze/CompF3_Report_Jun28.pdf?dl=0

- Incorporating *domain knowledge* into ML (*inductive bias*) can provide better task performance, better sample efficiency, smaller model size, interpretability and explainability, and robustness against domain shift
  - e.g. image classification is translation-invariant and some architectures respect that



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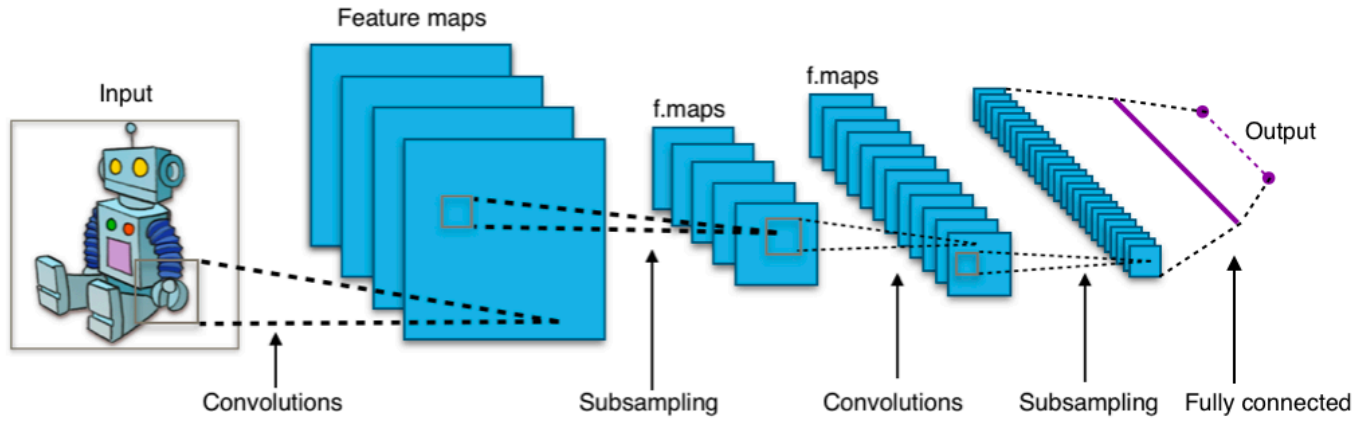

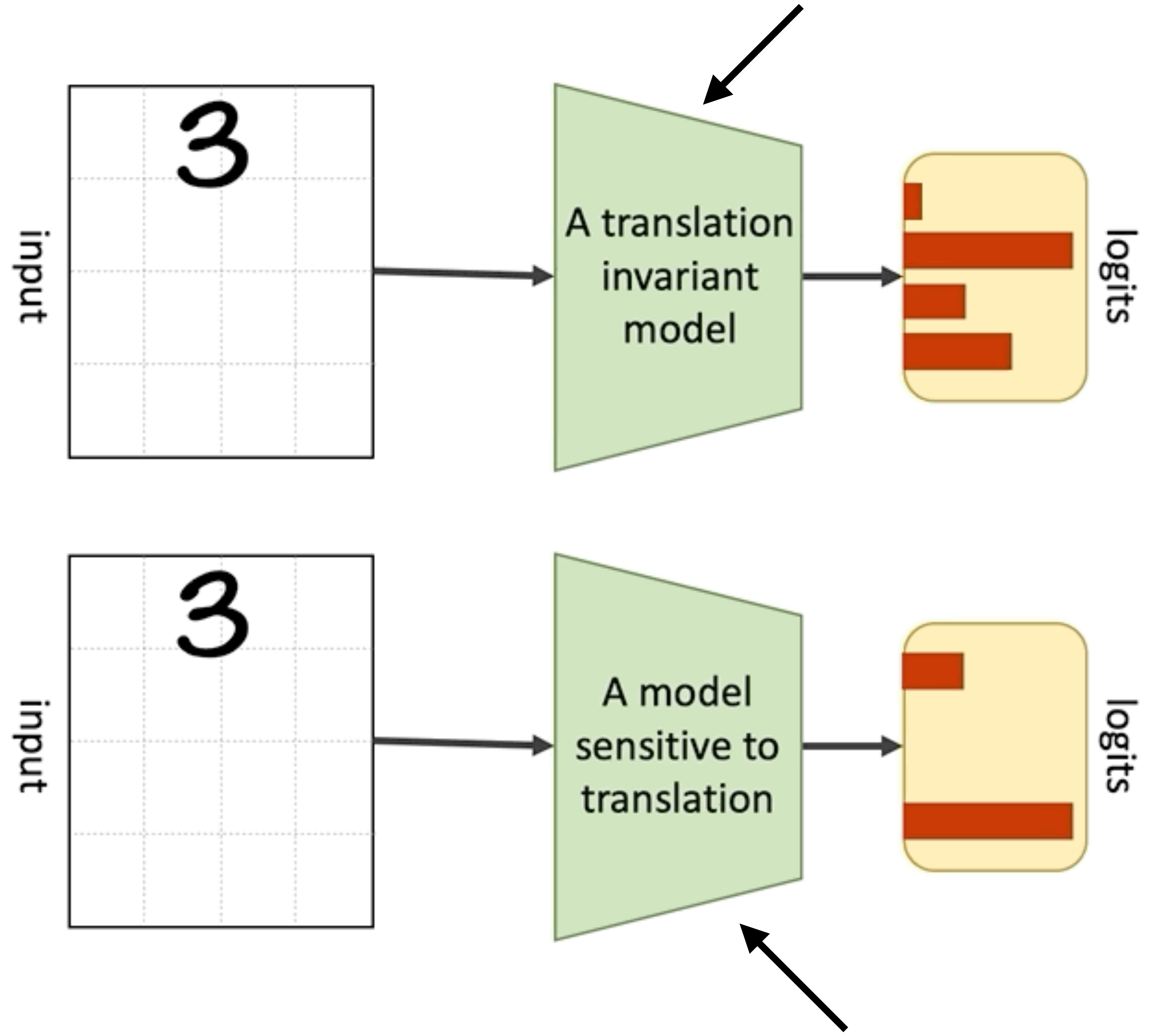

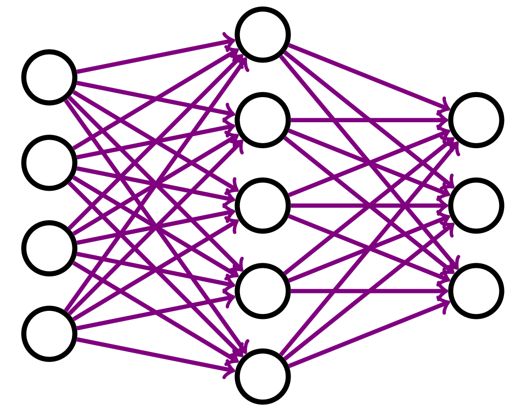

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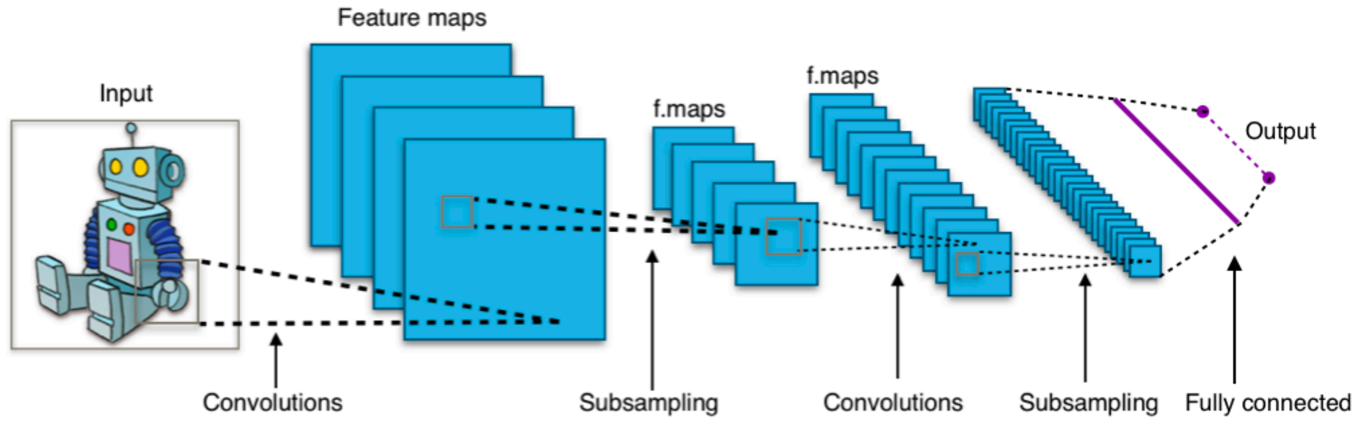

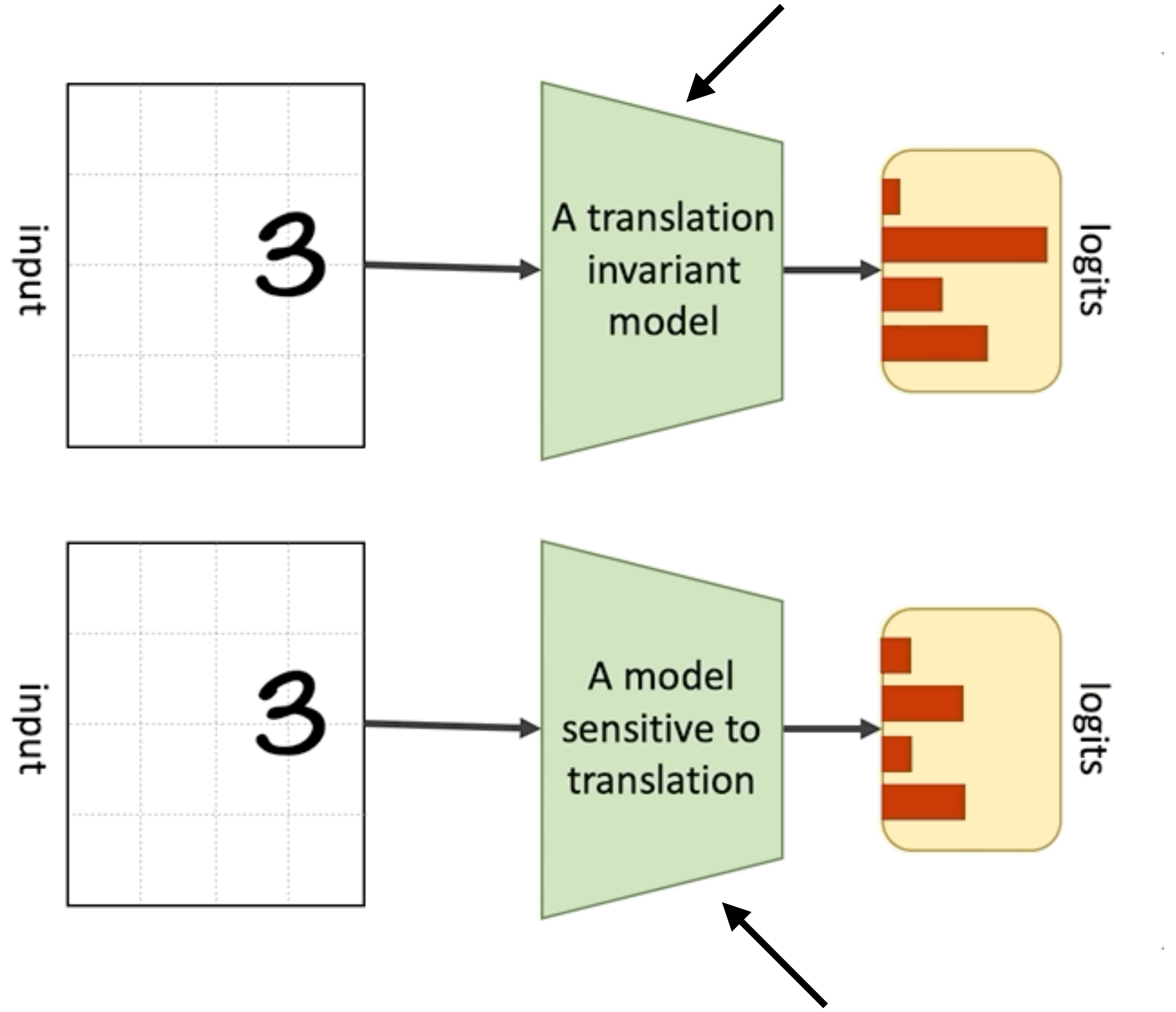

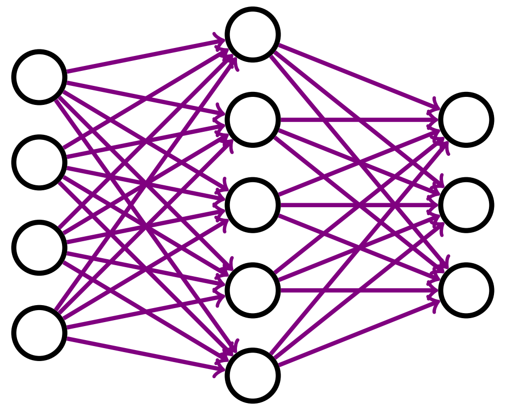

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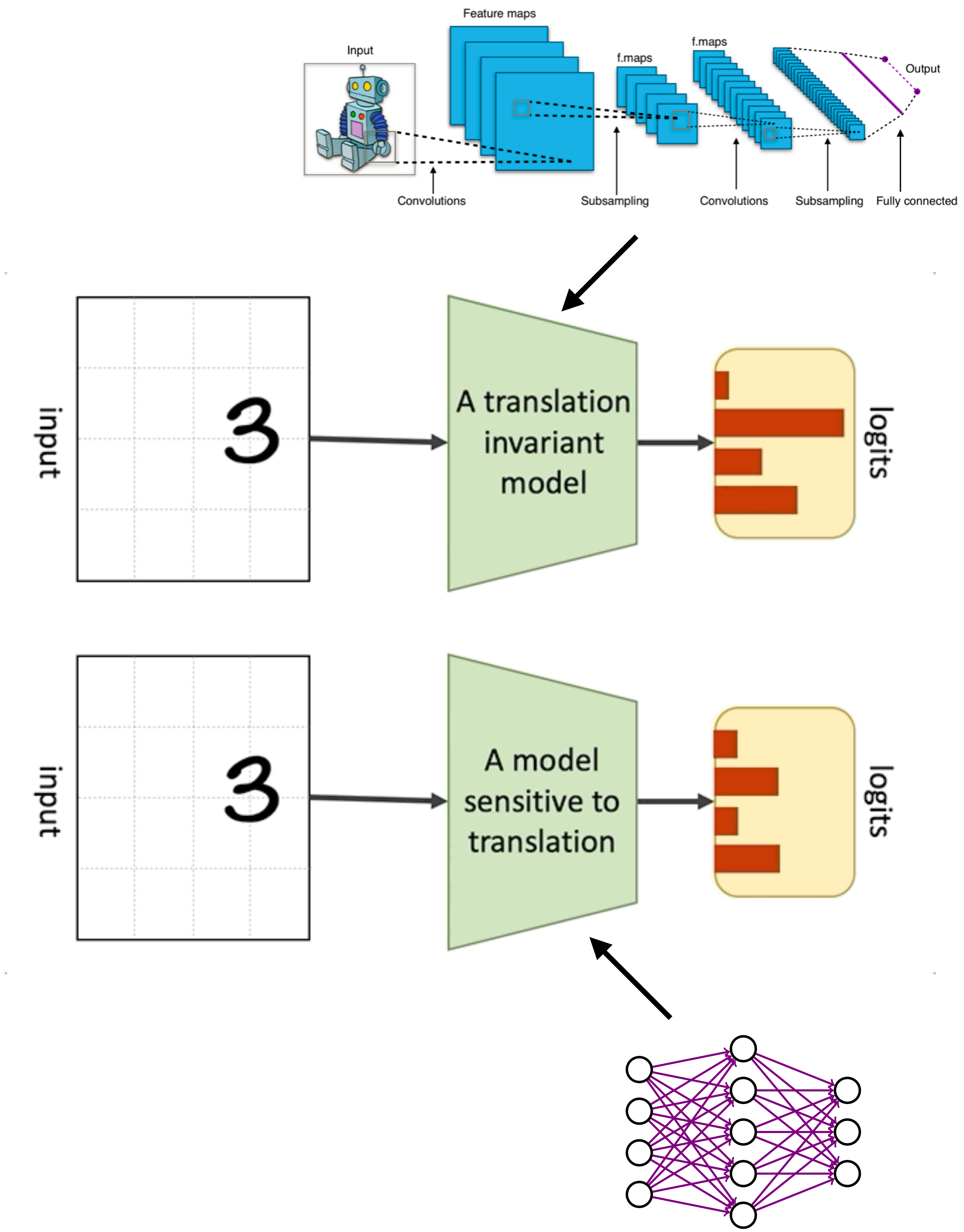
- Examples for HEP include:
  - Graph data representations
  - Physics-constrained ML
  - Symmetry-equivariant networks



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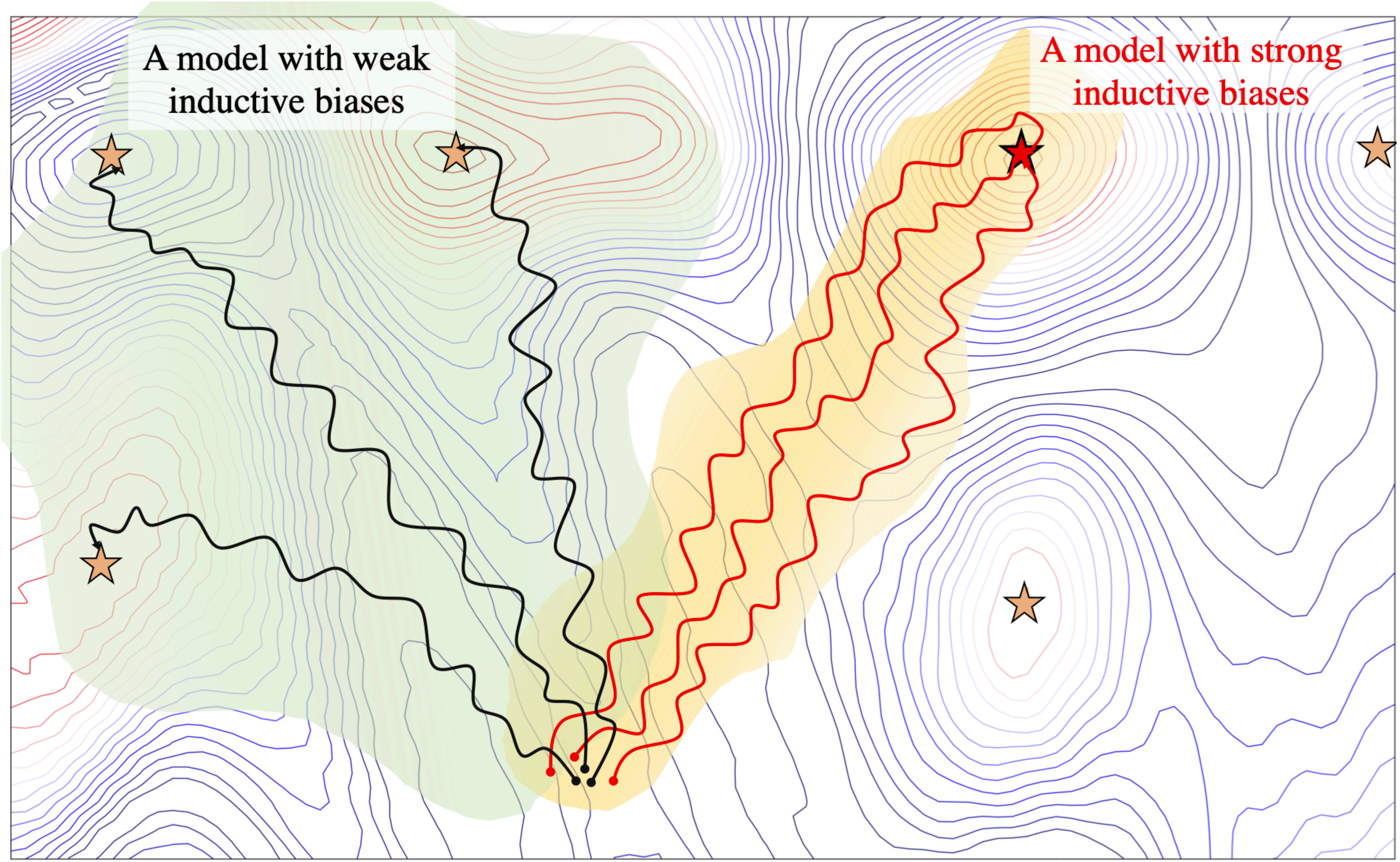

HEP DATA REPRESENTATIONS

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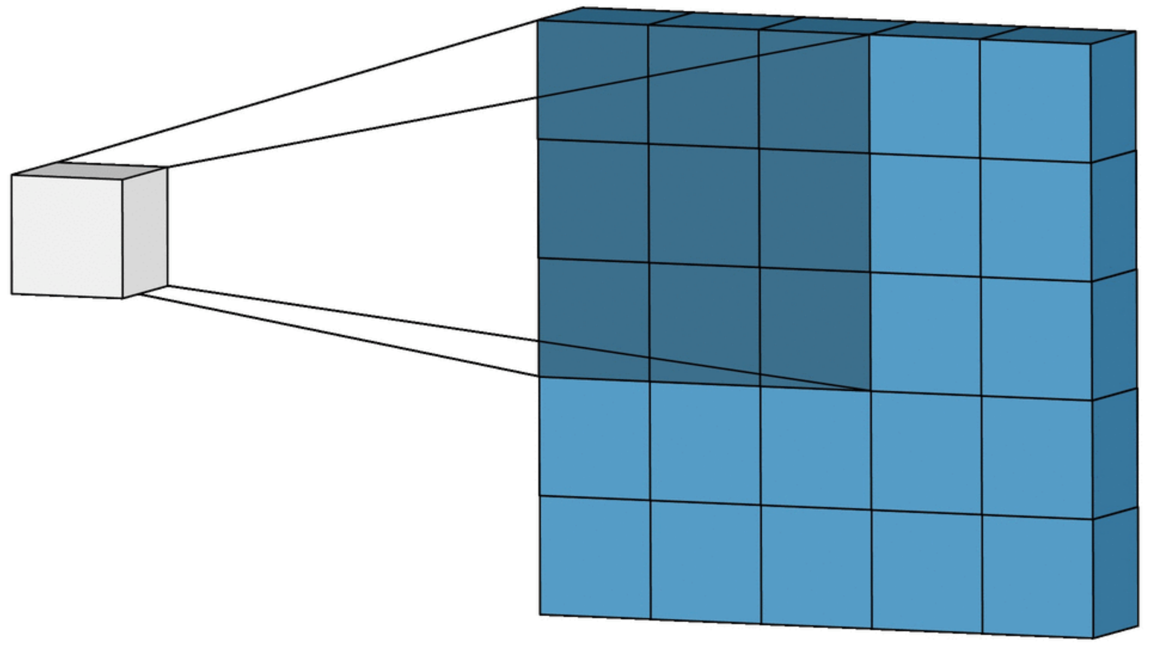

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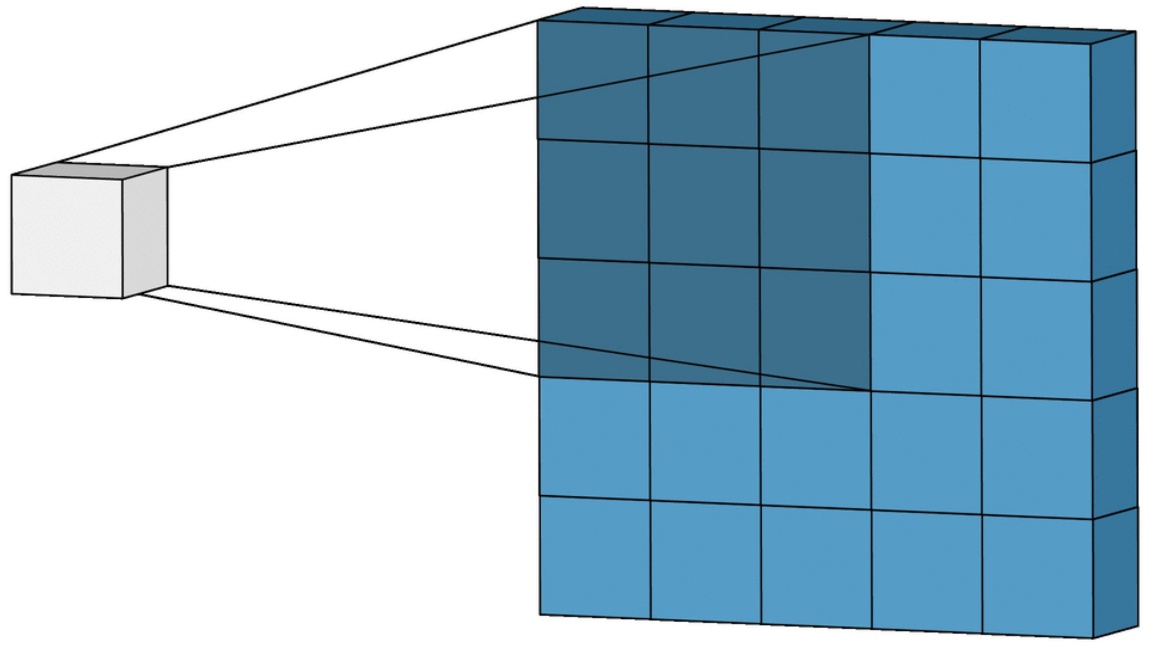
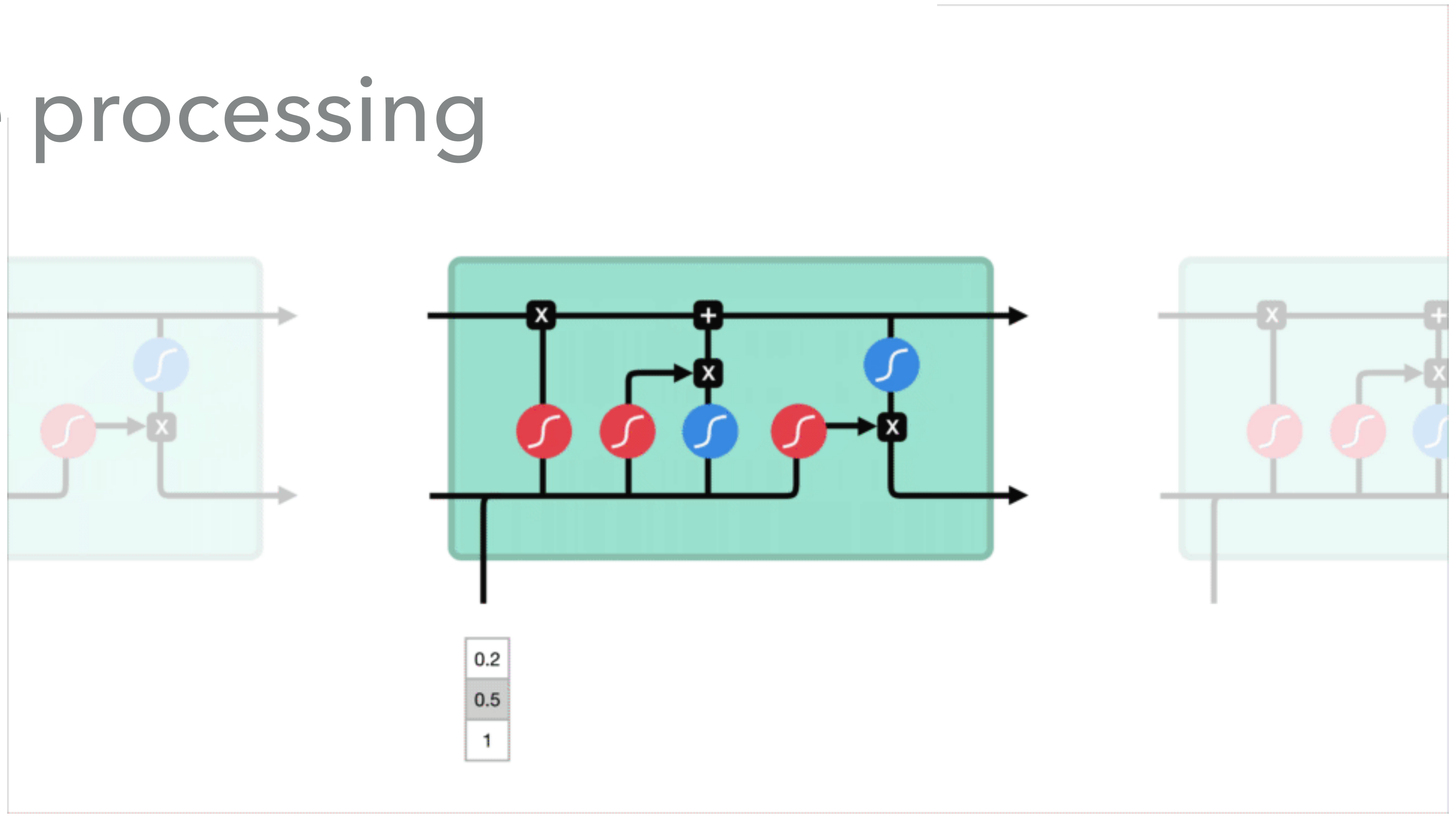


  - RNNs for language processing



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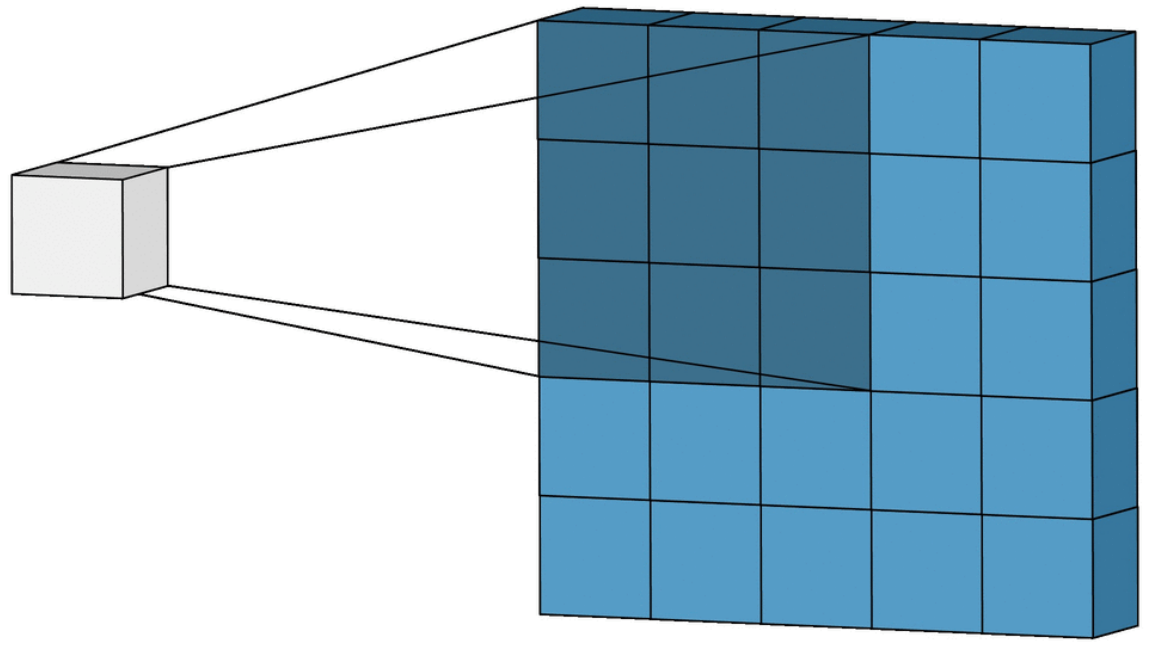

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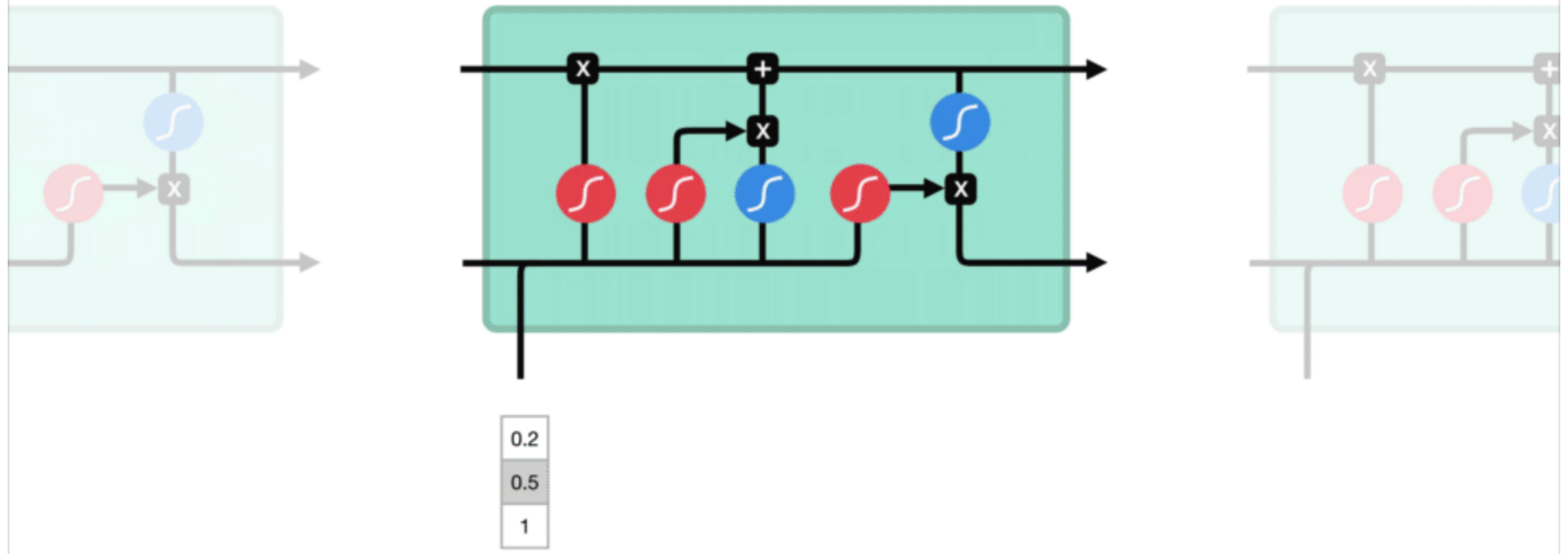

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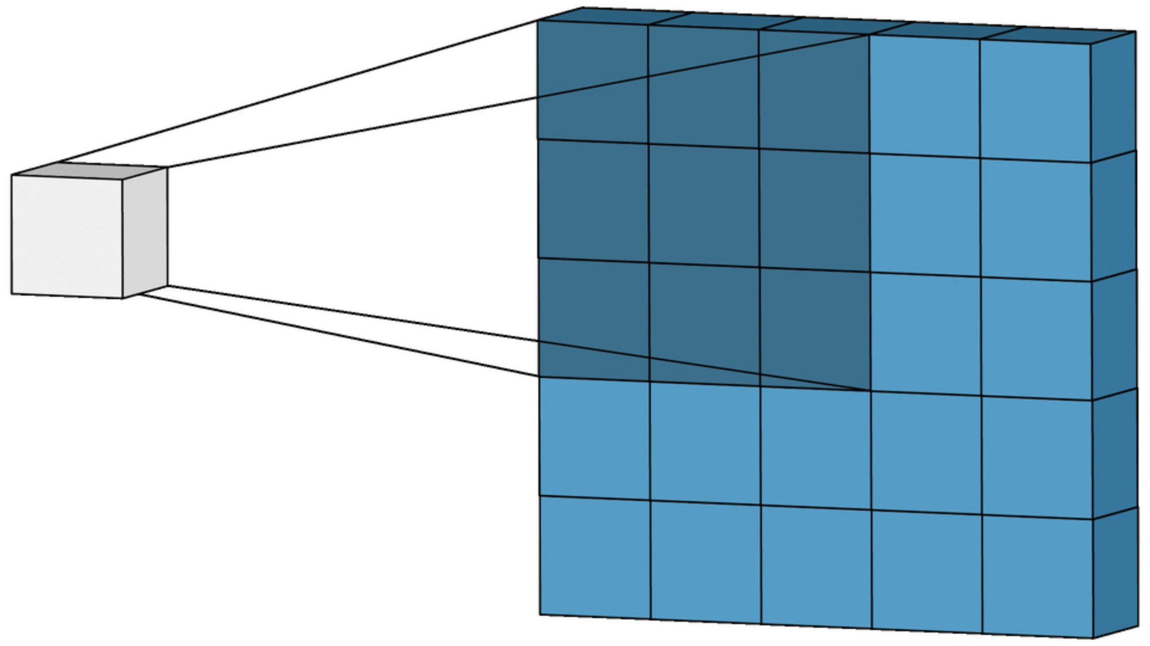

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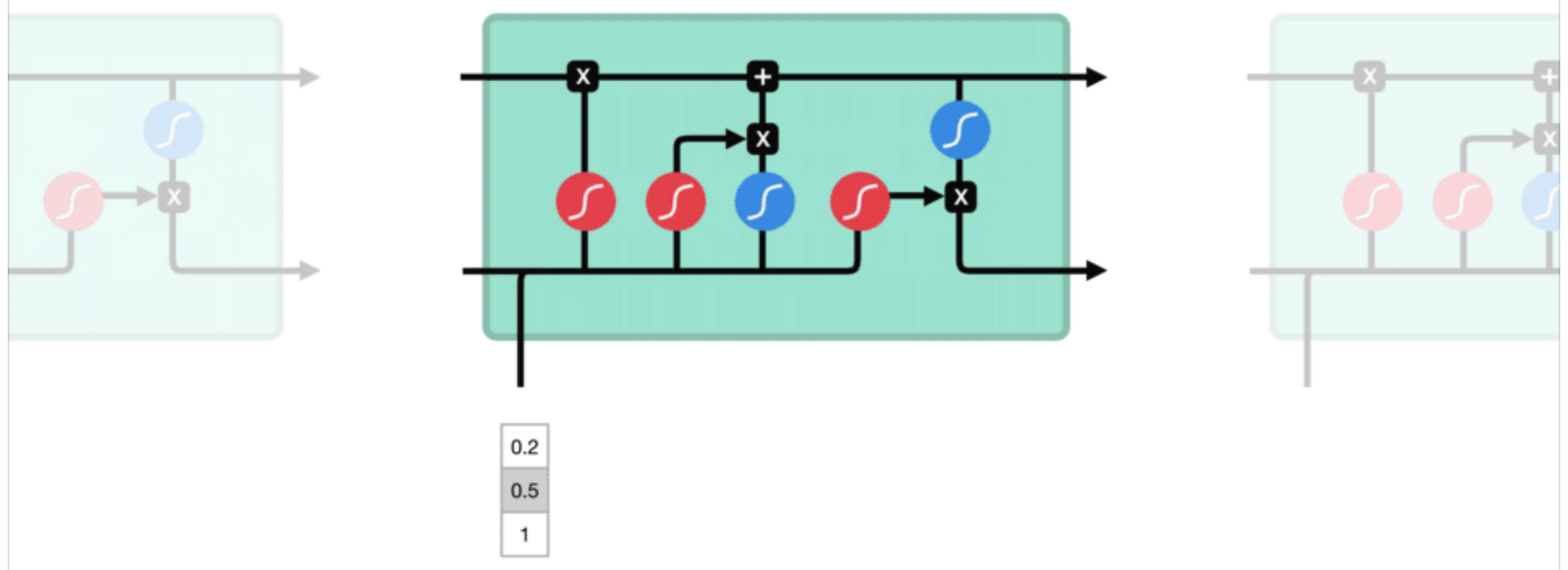
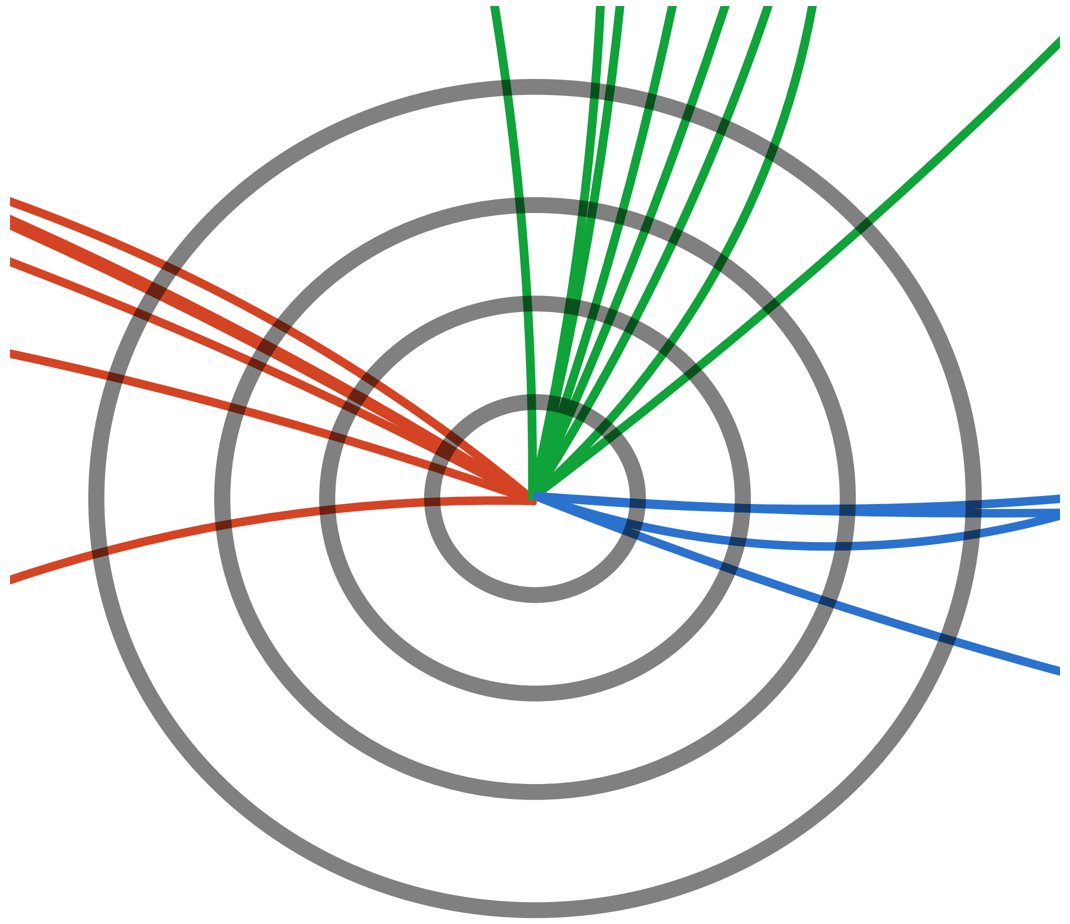


- Distributed unevenly in space
- Sparse
- Variable size
- No defined order
- Interconnections



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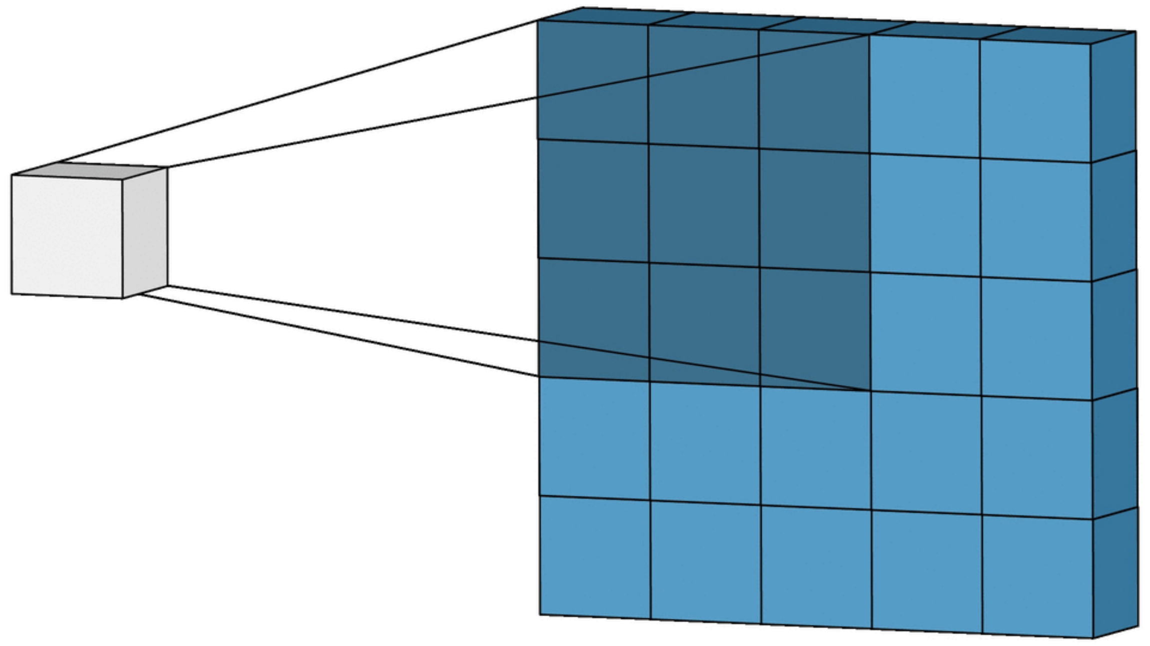

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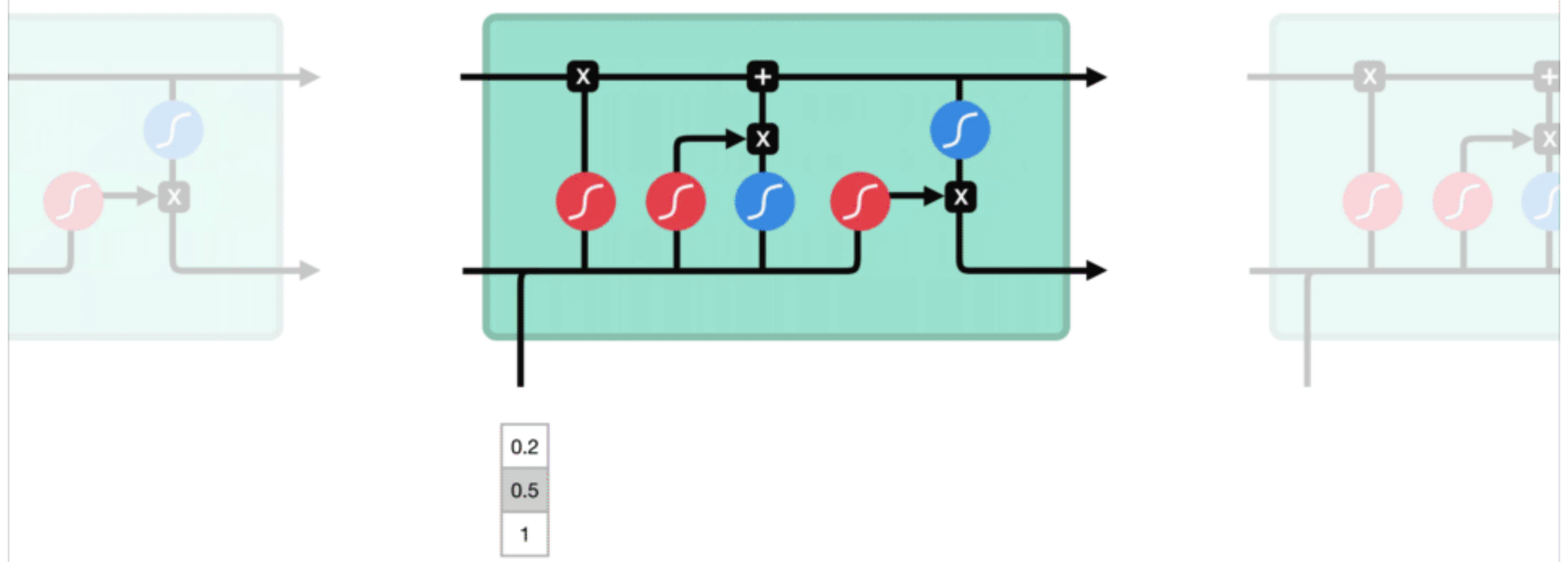

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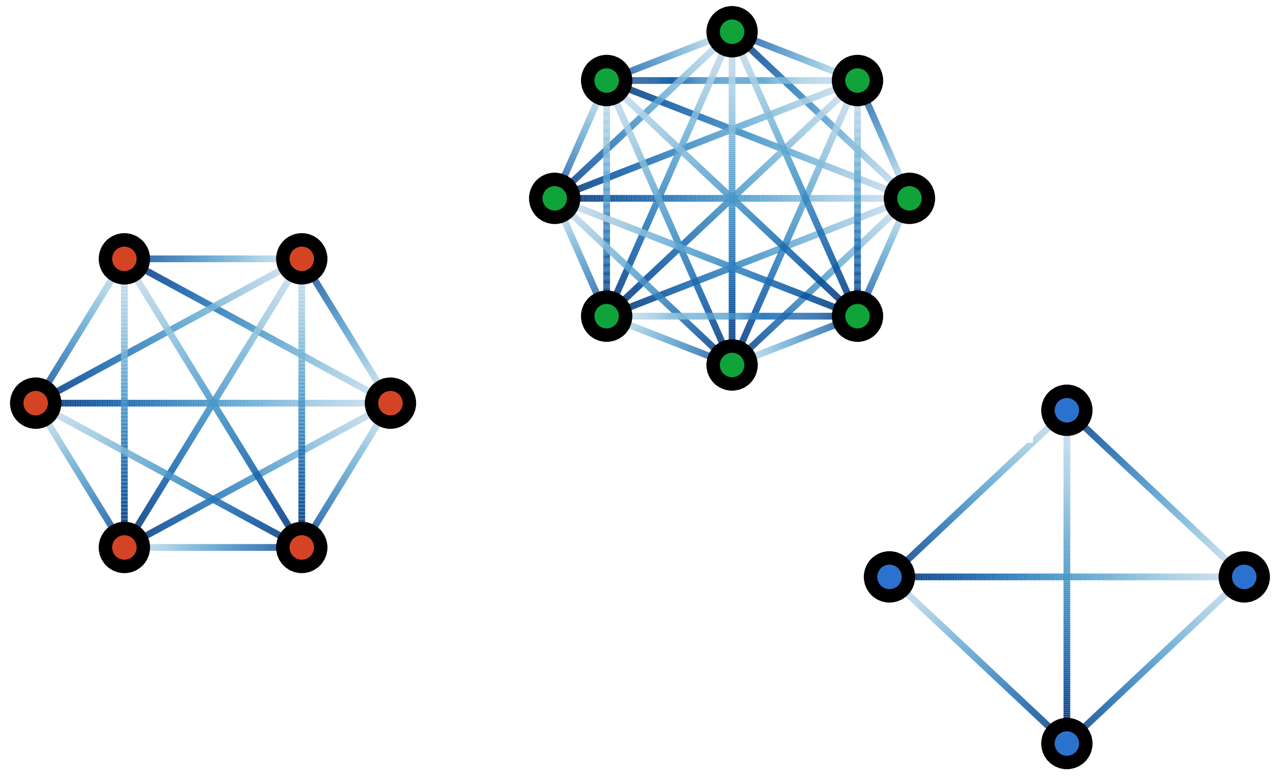

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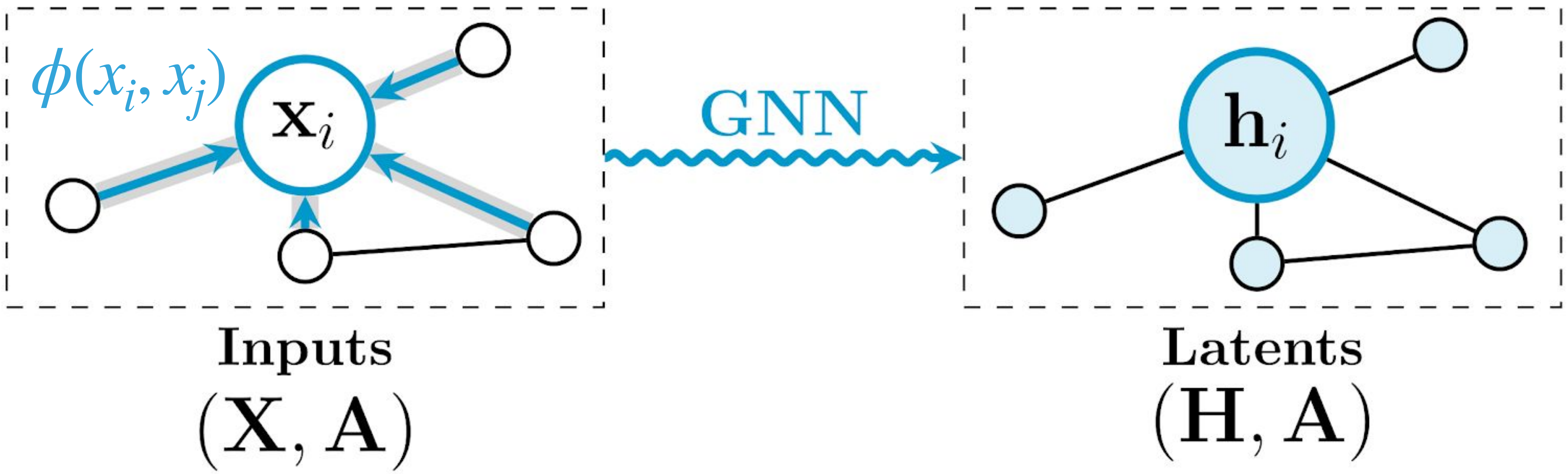
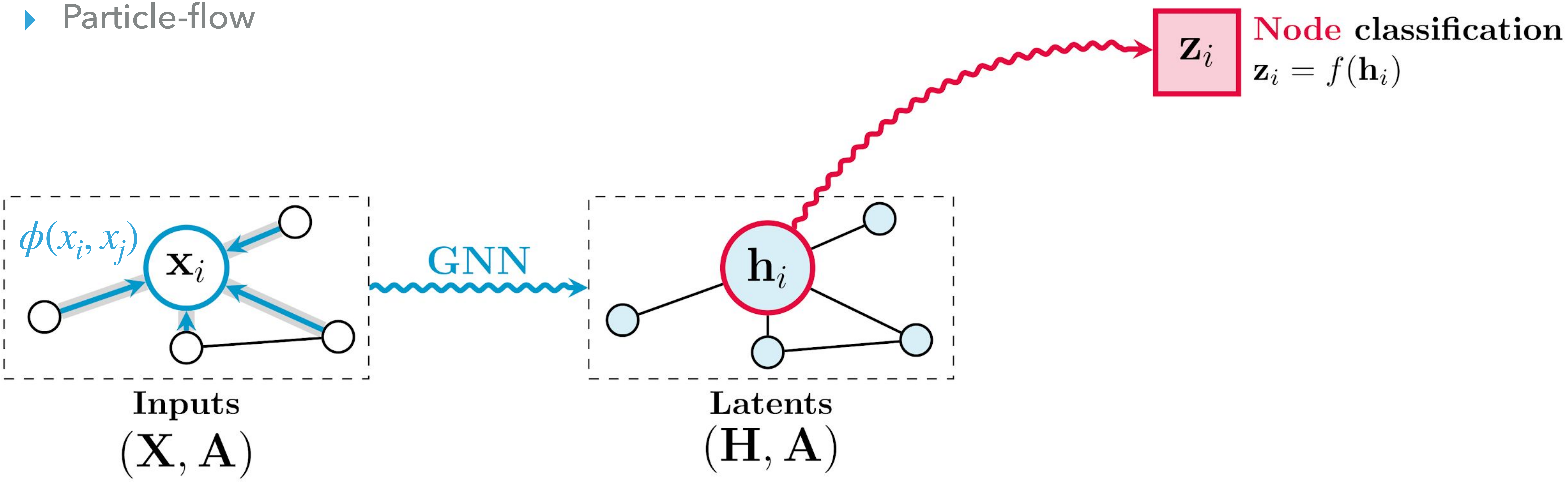
GRAPH NEURAL NETWORKS IN HEP



GRAPH NEURAL NETWORKS IN HEP

- Node-level tasks
  - Identify "pileup" particles
  - Particle-flow



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- Graph-level tasks
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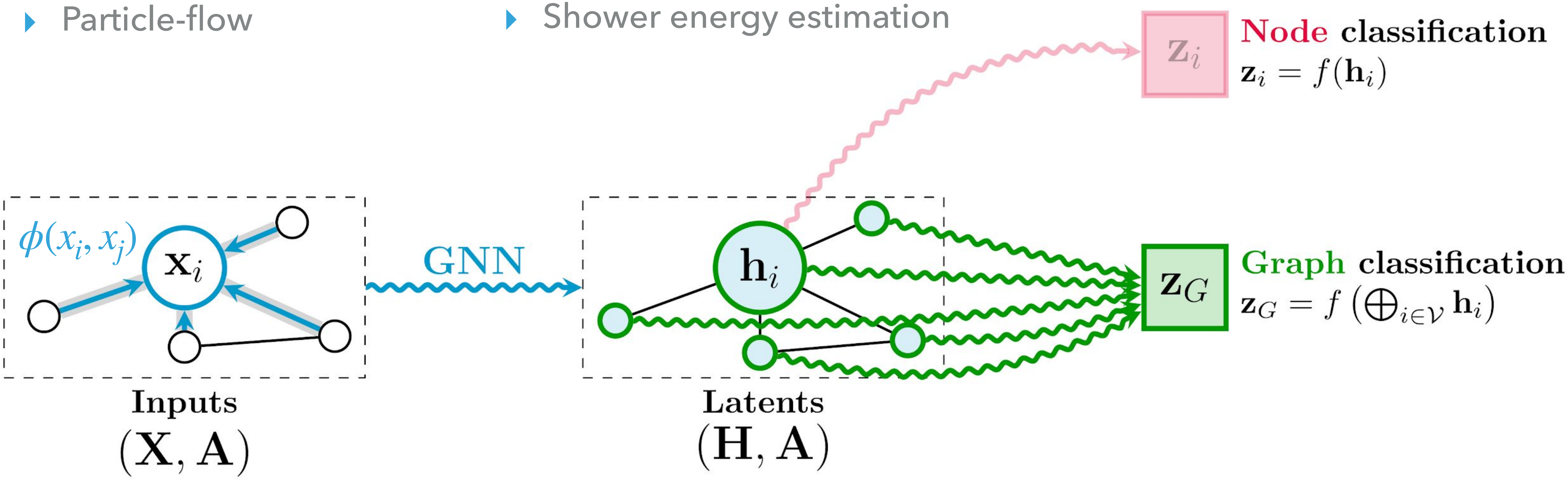
  - Shower energy estimation



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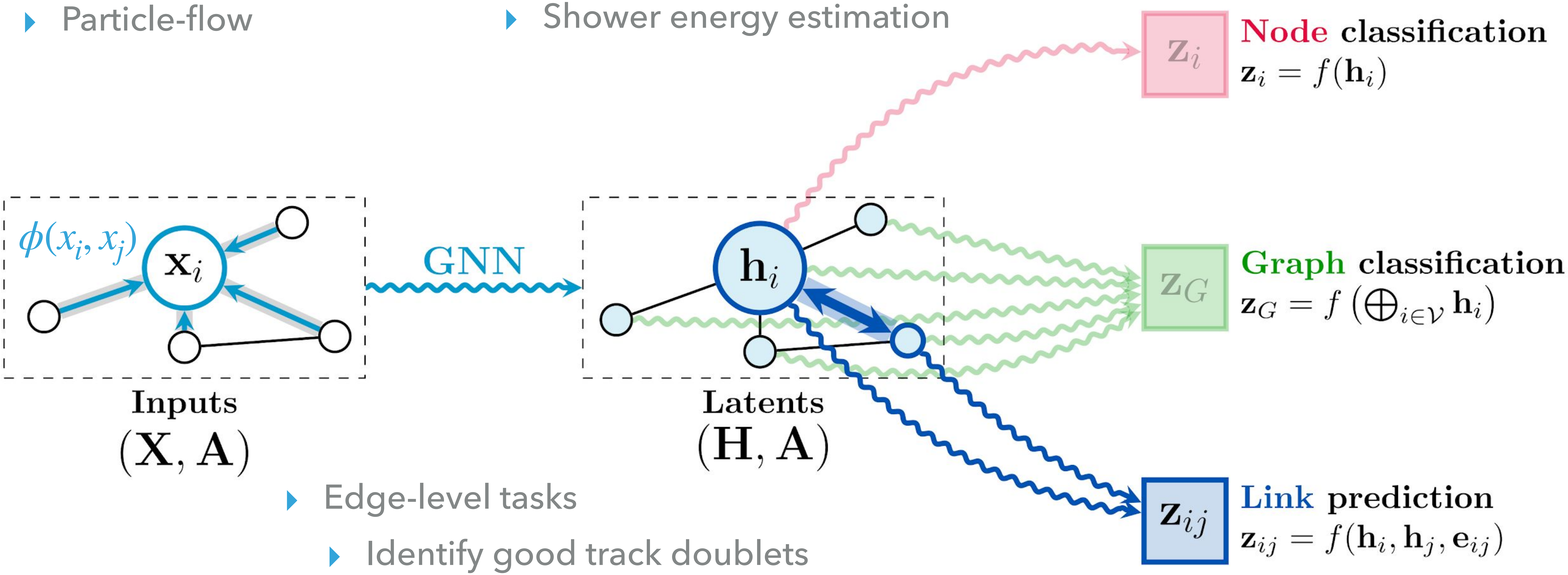
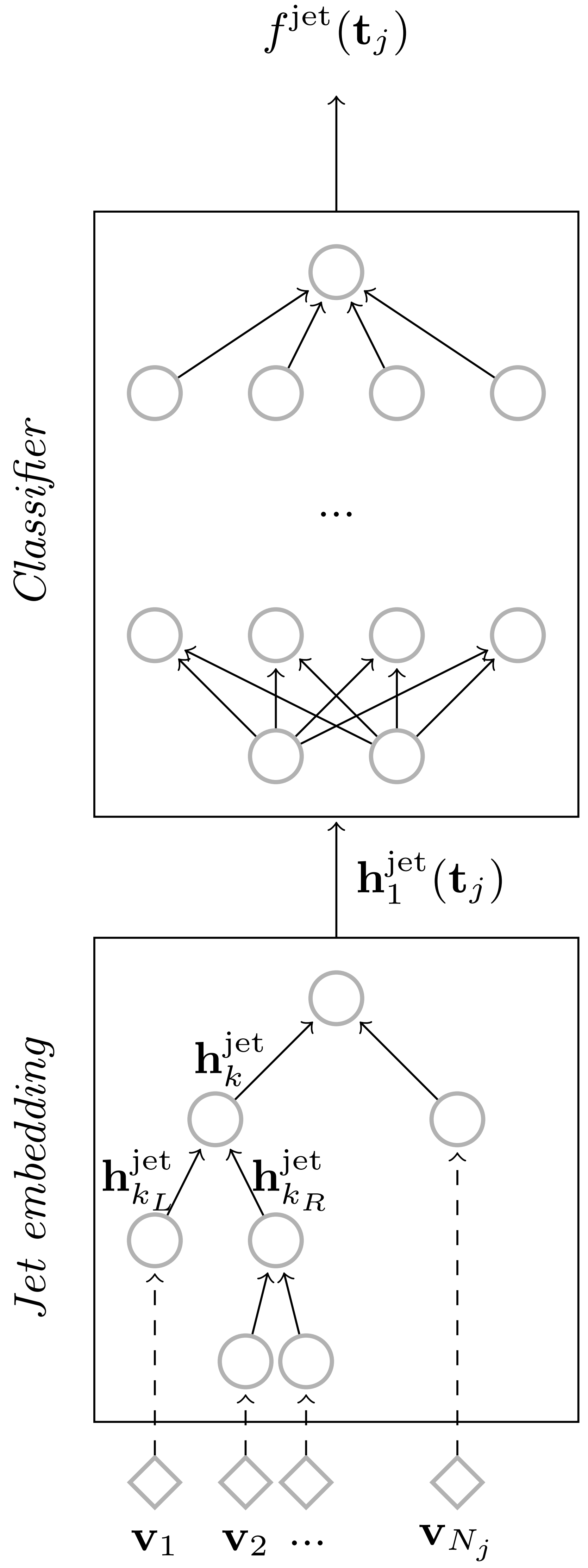


- Edge-level tasks
  - Identify good track doublets
  - Secondary vertex reconstruction

PHYSICS-CONSTRAINED ML

- Physics-motivated architectures like
  - QCD-aware recursive and graph networks



arXiv:1702.00748

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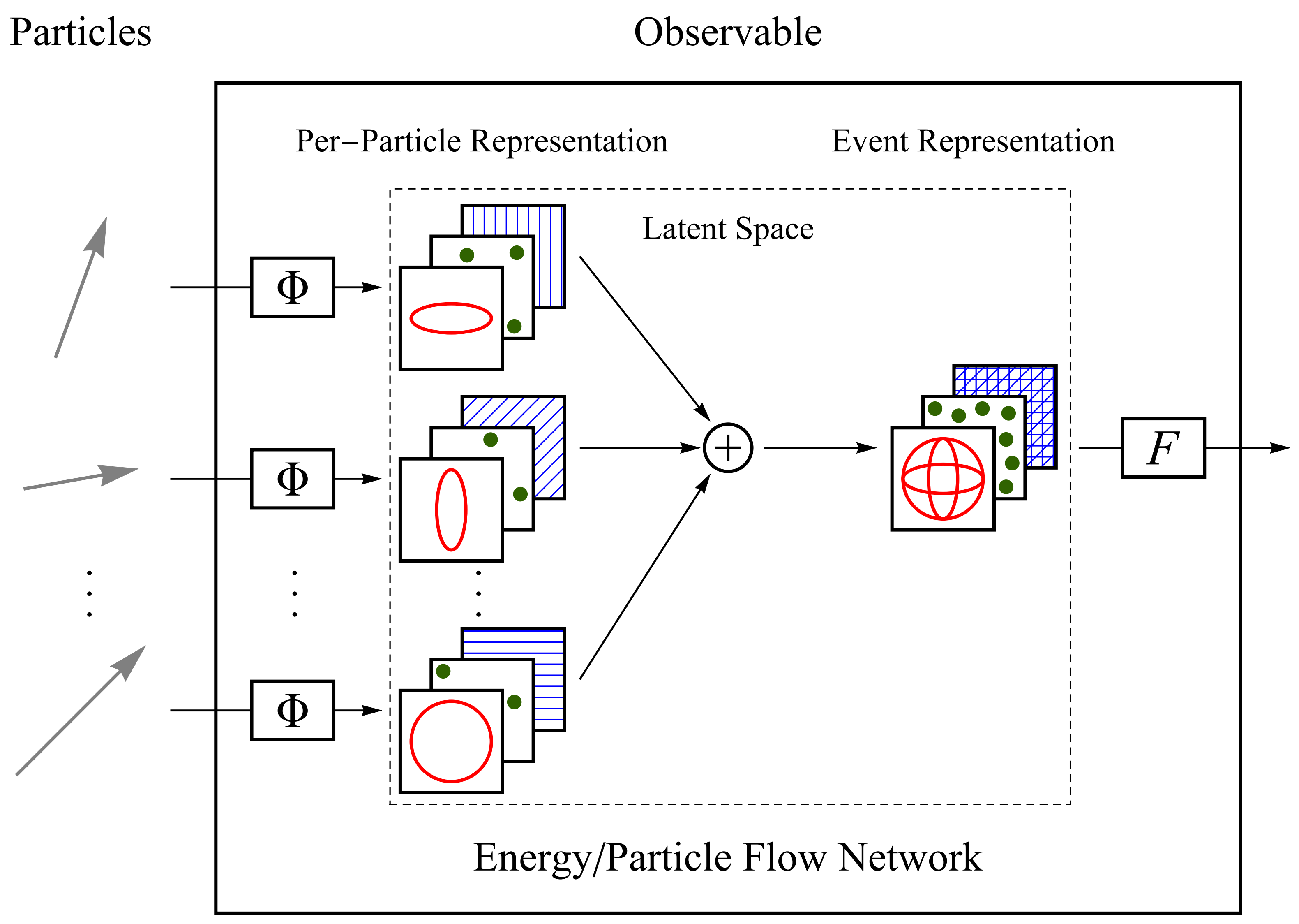

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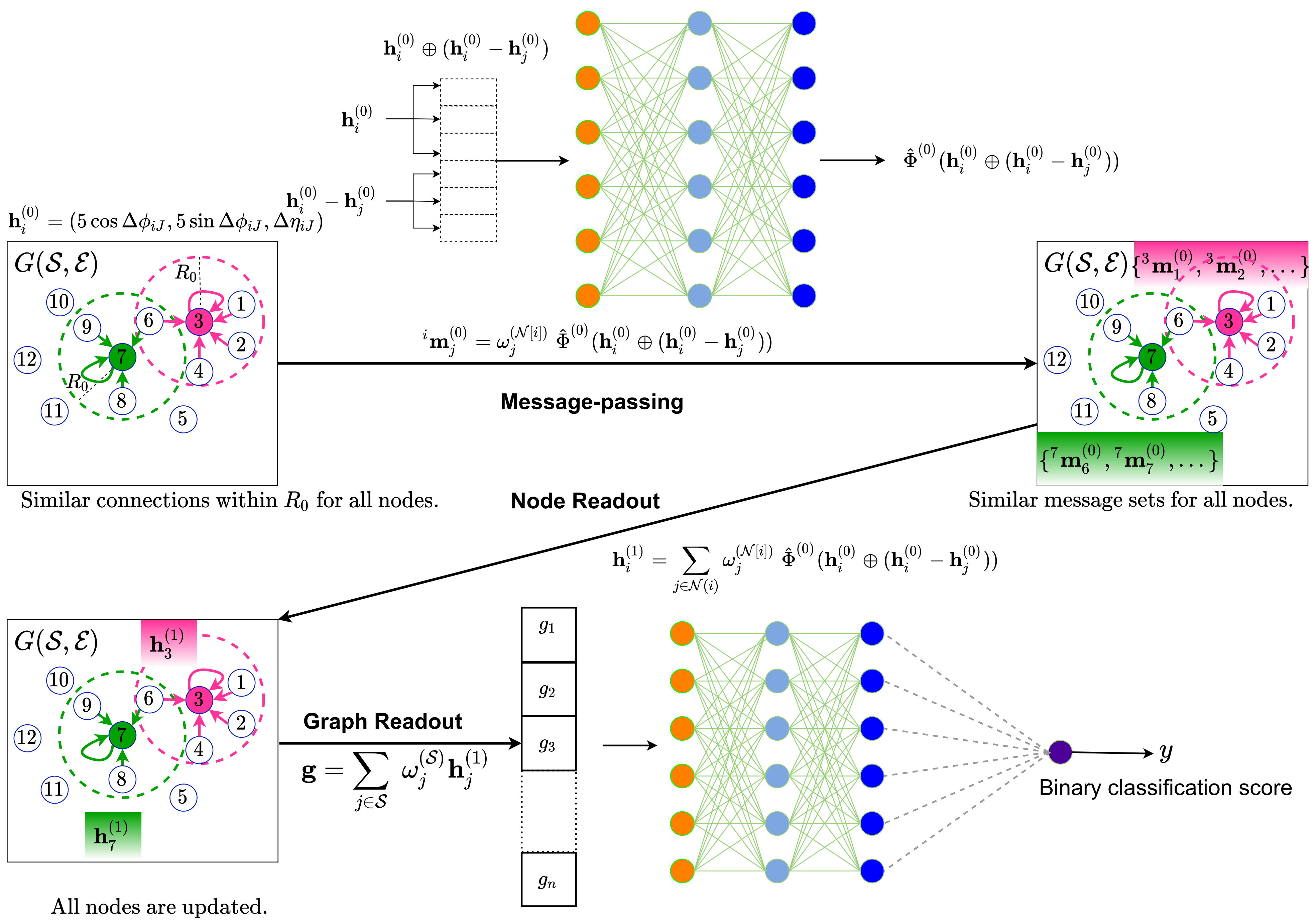

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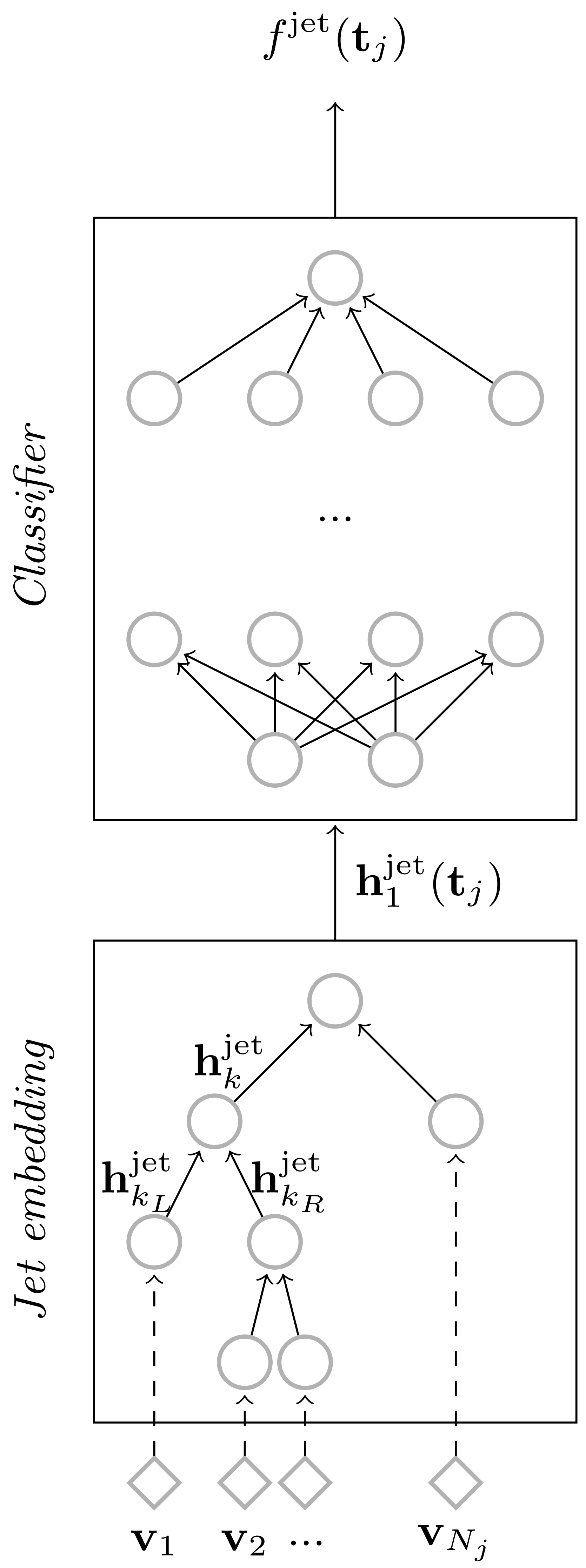

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PHYSICS-CONSTRAINED ML

- Physics-motivated architectures like
  - QCD-aware recursive and graph networks
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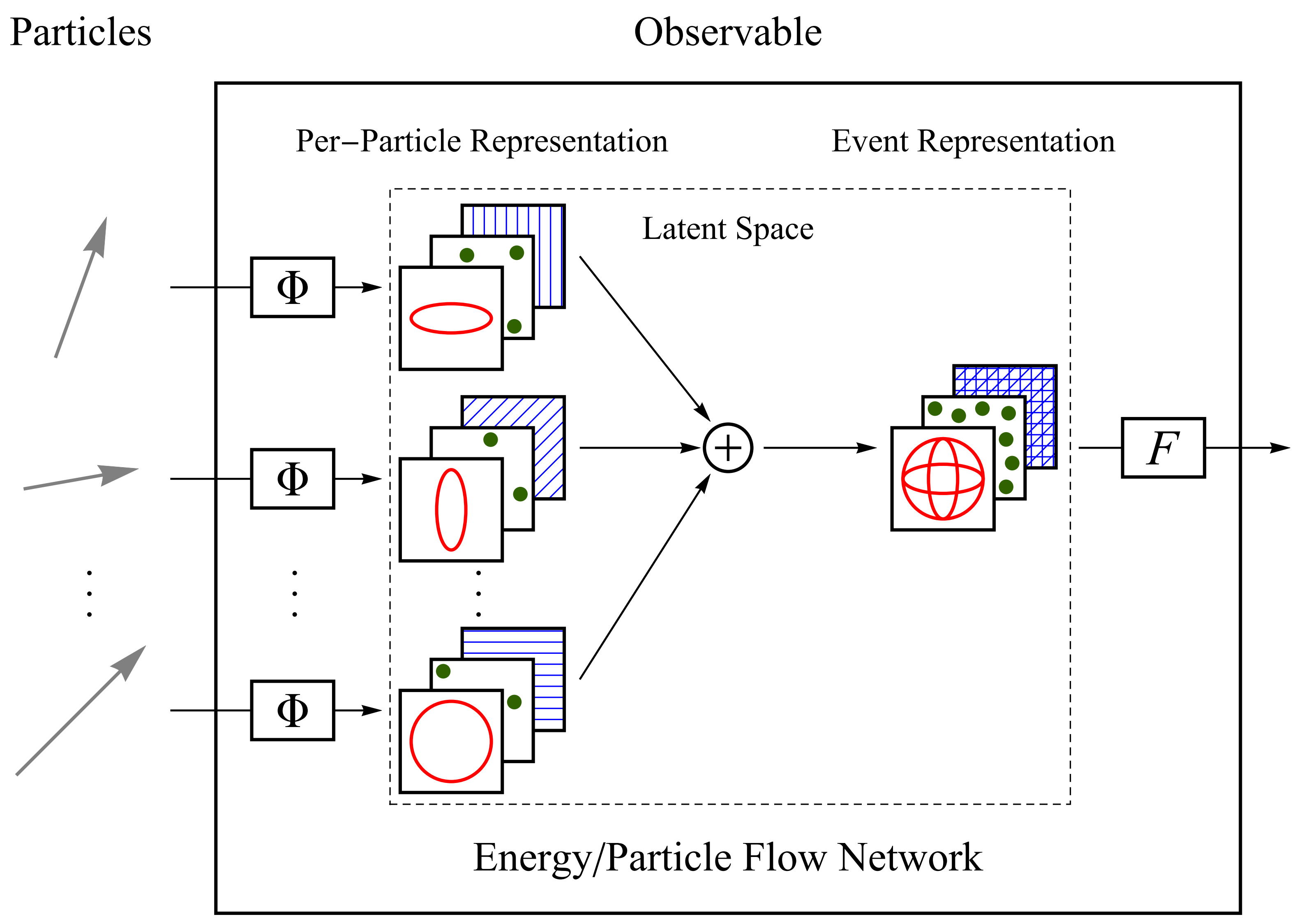
- Potentially more robust, interpretable, easier to quantify uncertainties
- Other constraints: speed, size, etc.



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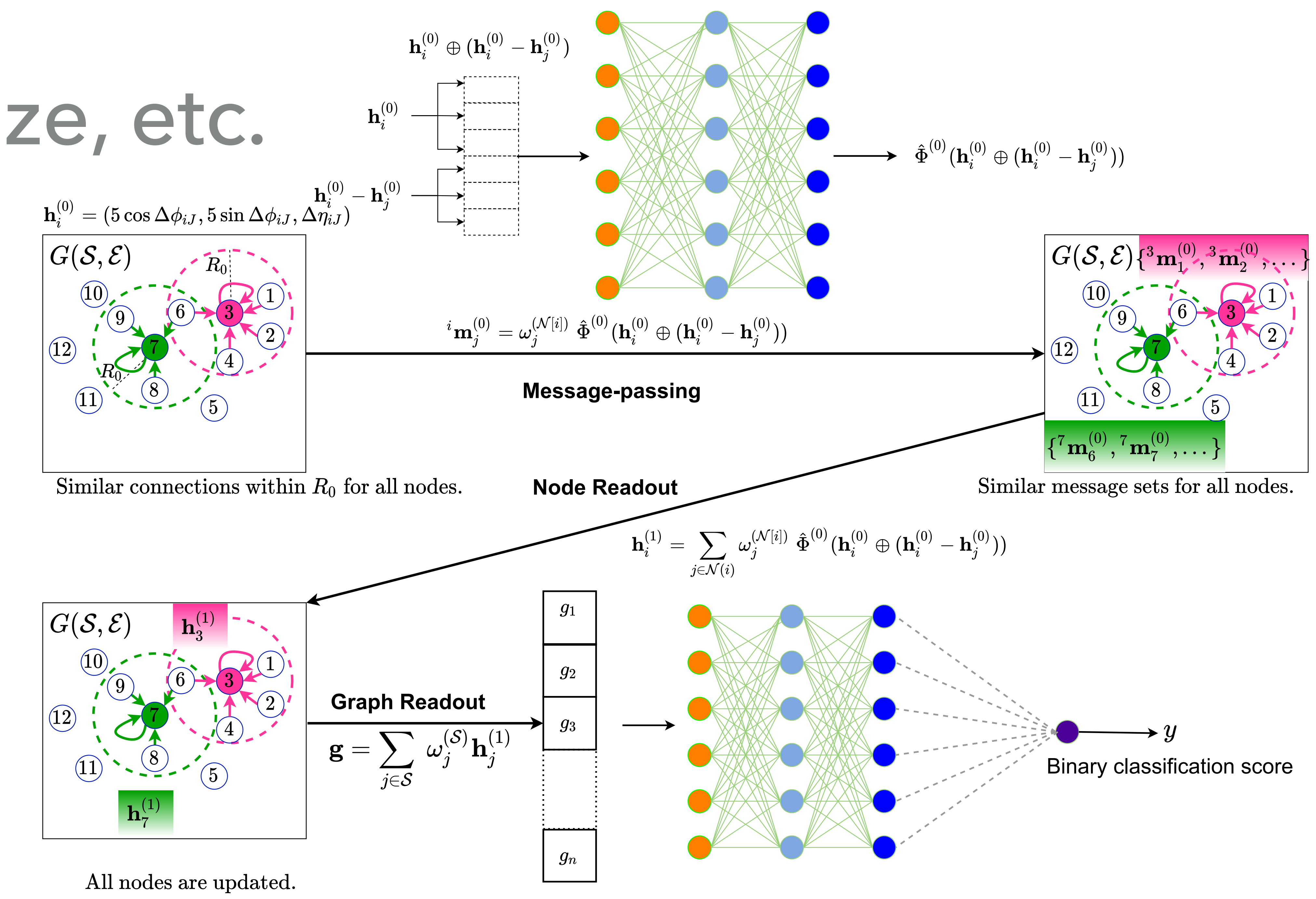

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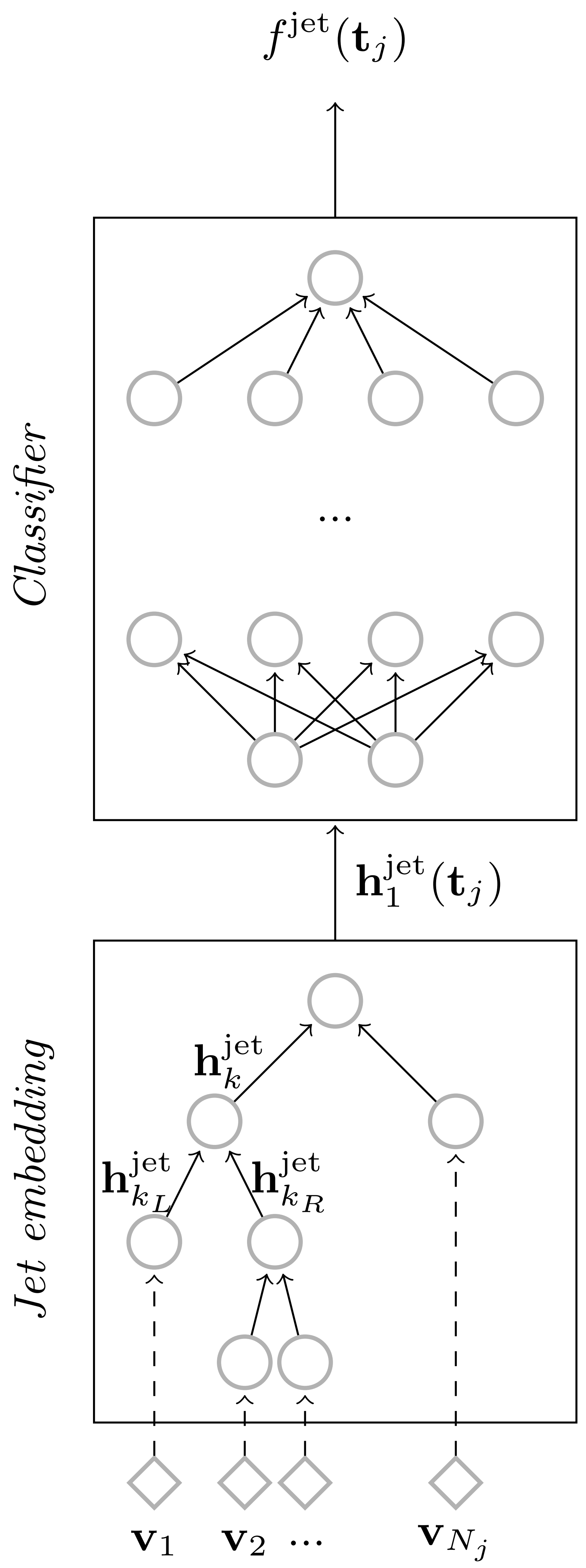

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SYMMETRY-EQUIVARIANT NETWORKS

- Symmetry-equivariant networks, e.g. for Lorentz symmetry
  - More economical (fewer, but more expressive parameters), interpretable, and trainable

Invariance

$f(\rho_g(x)) = f(x)$

Equivariance

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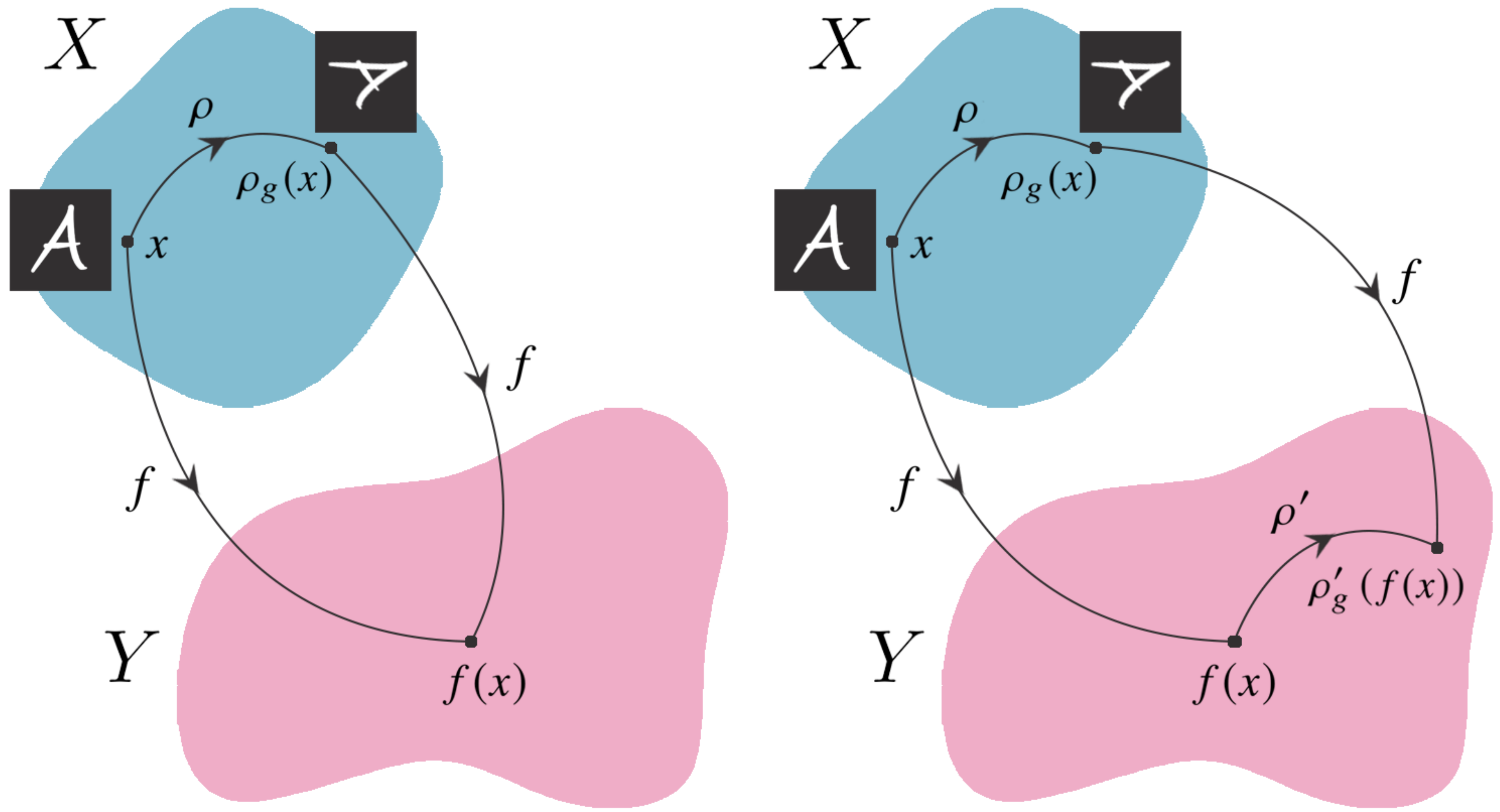

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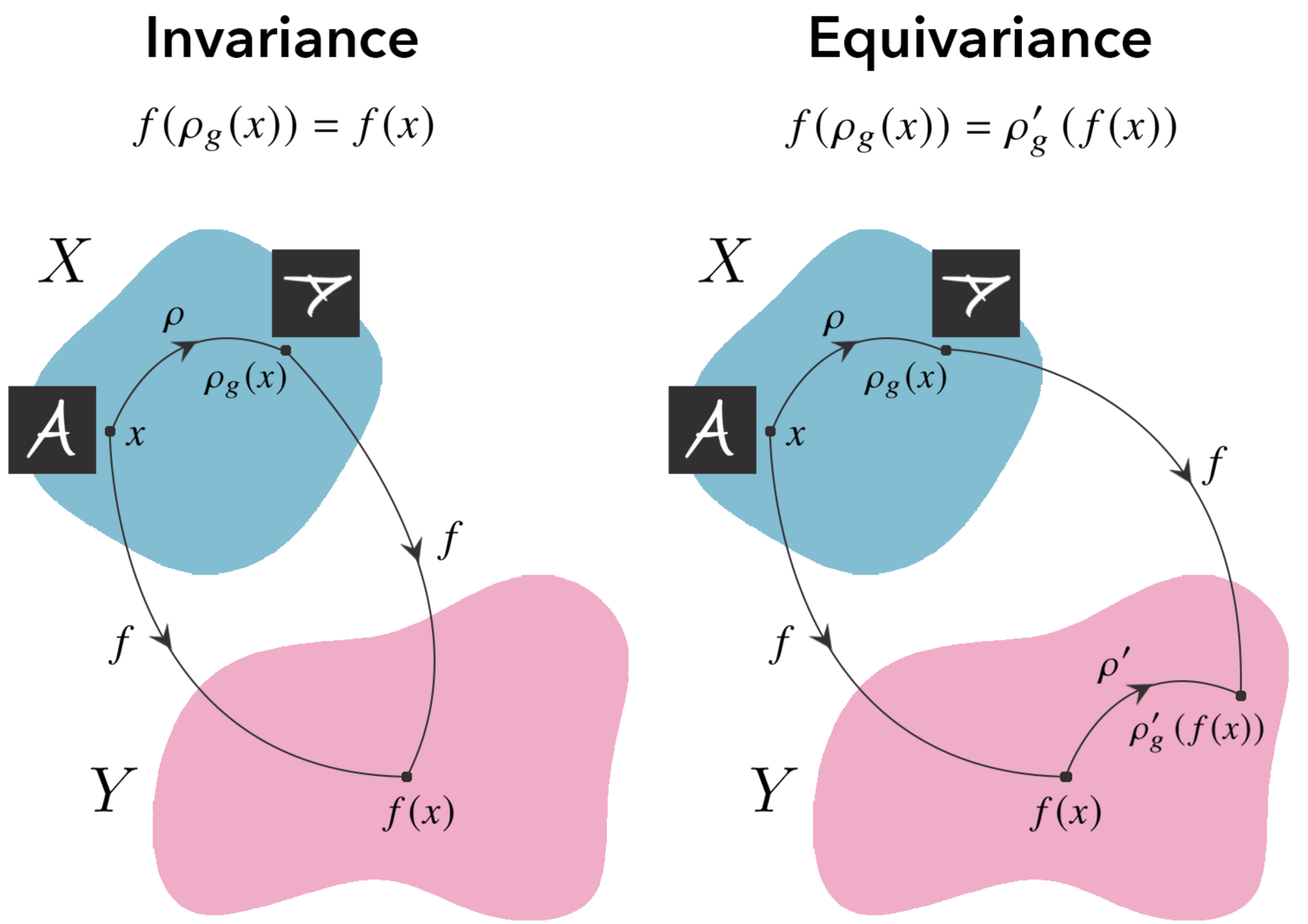

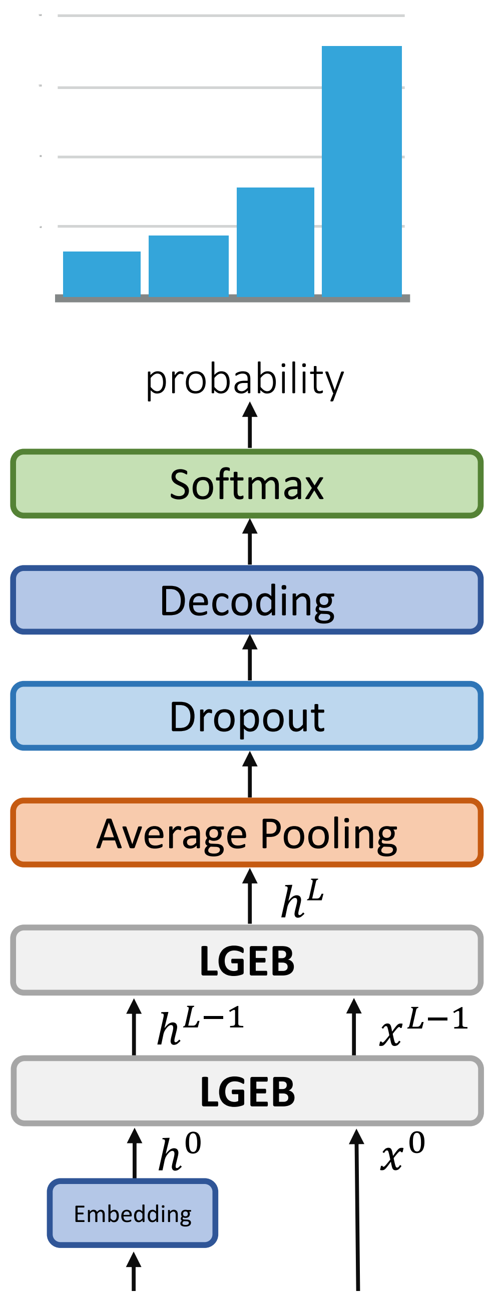

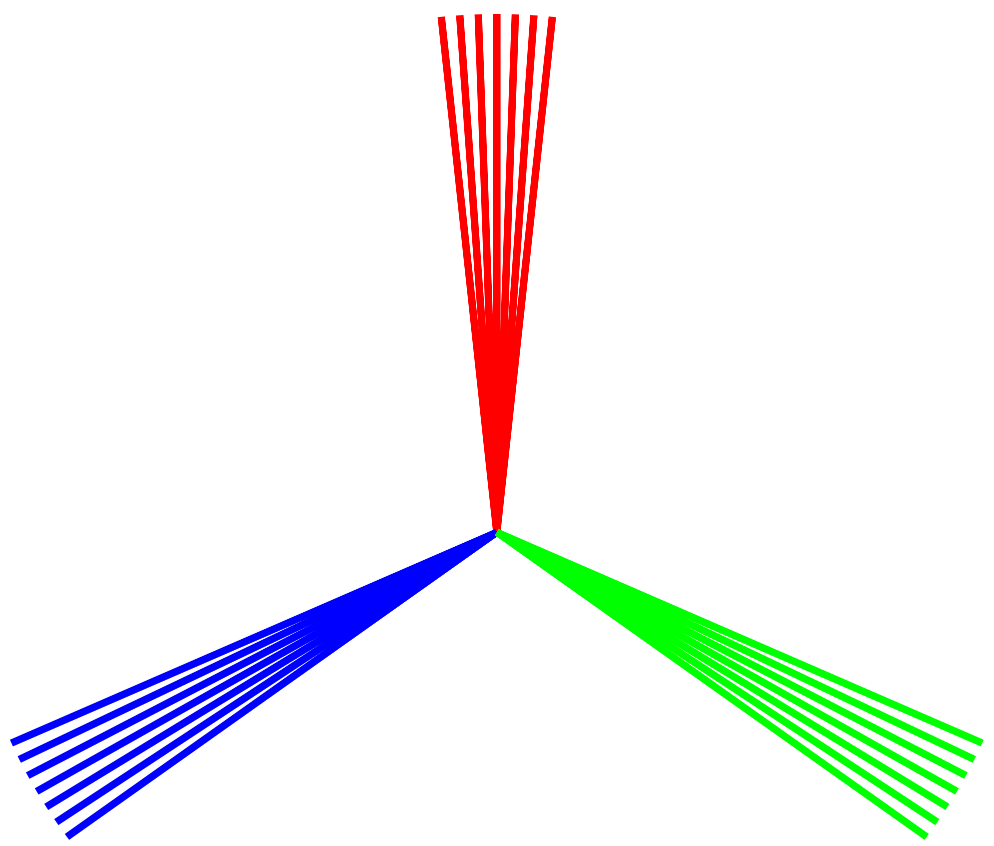

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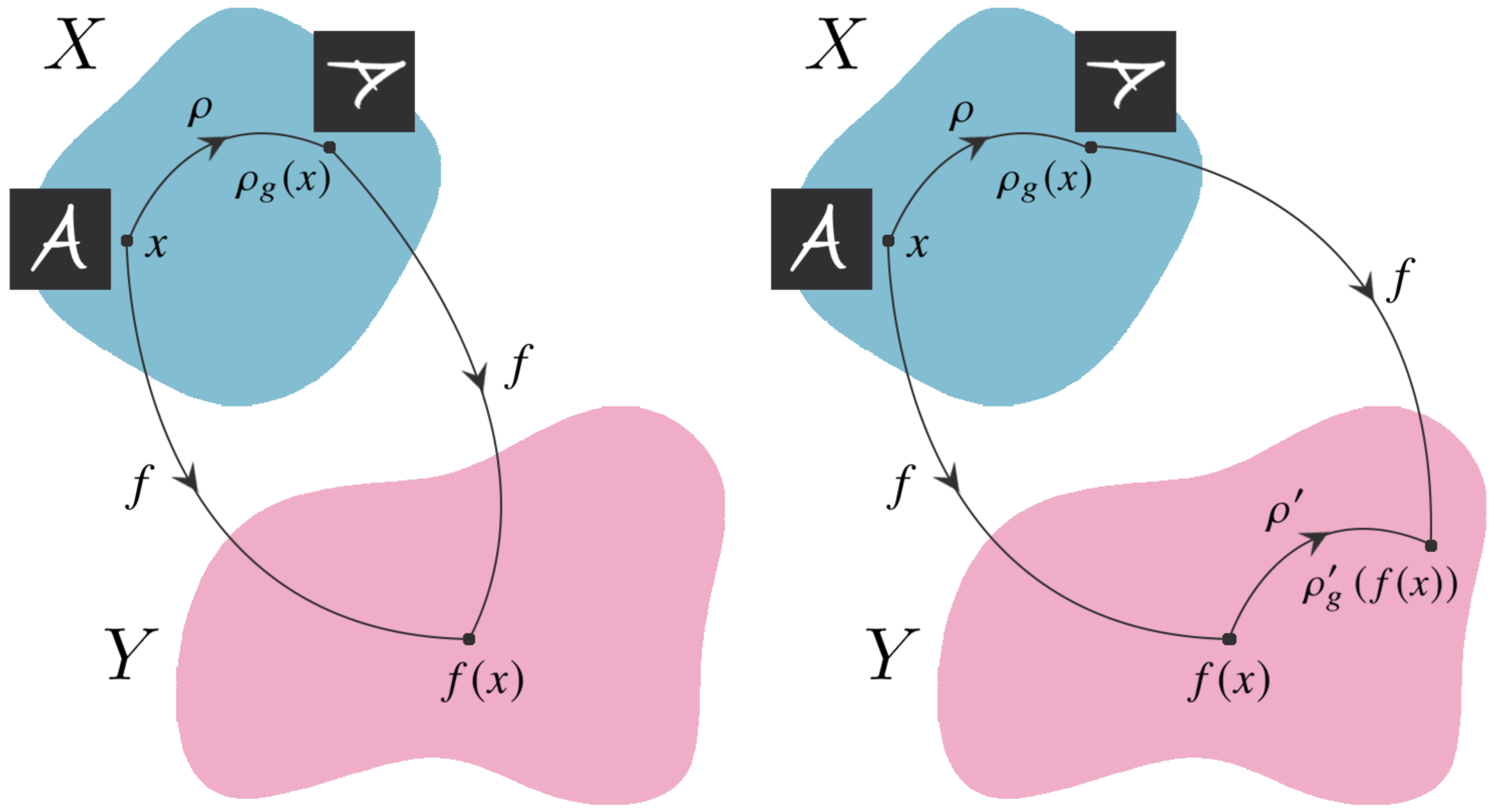

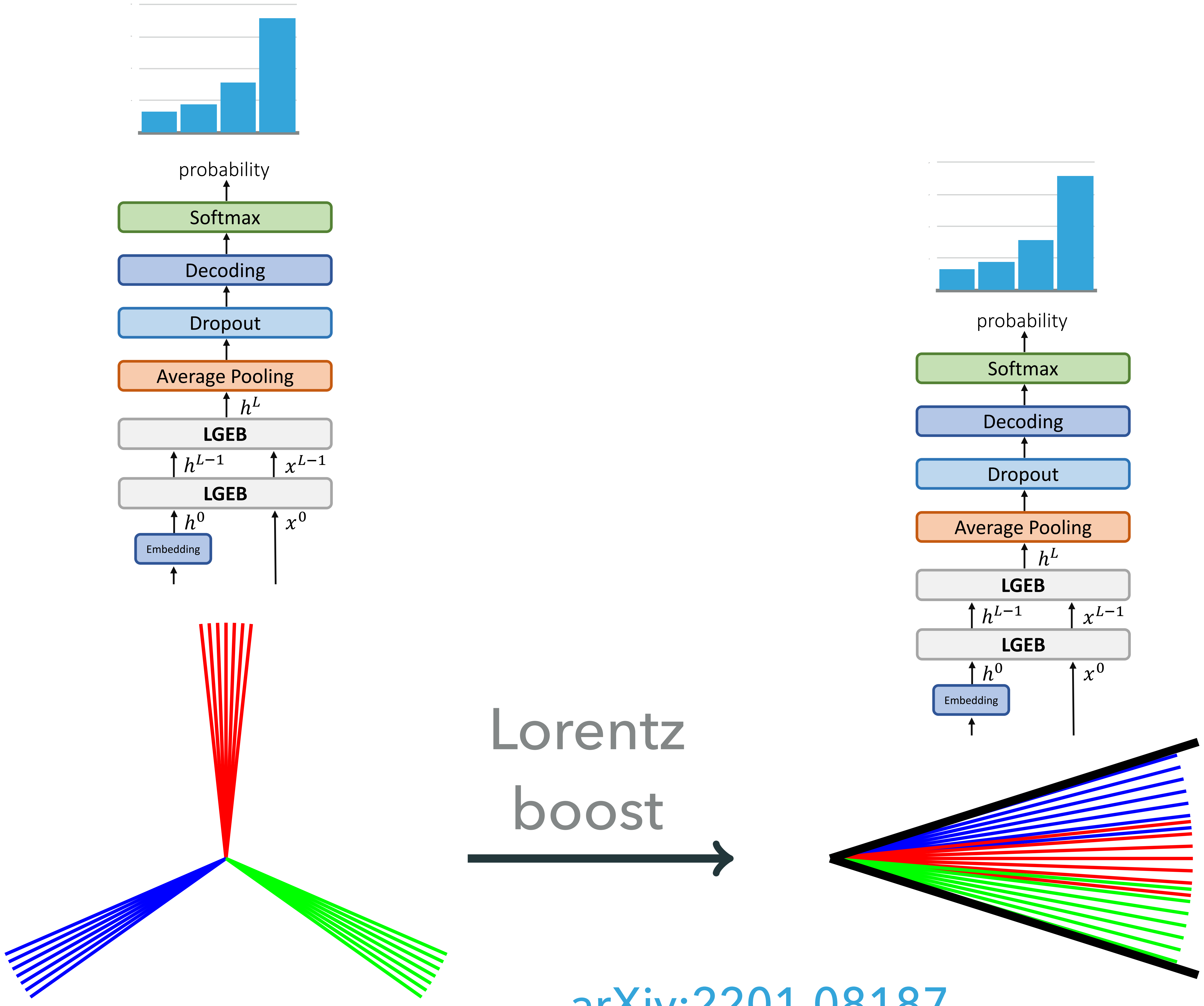

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- Encoding key physics knowledge results in quicker learning with smaller training samples
- Recommendations:
  - Dedicated support and review criteria that helps research along this category
  - Defined metrics concerning the strengths of physics-specific ML (e.g. sample efficiency, learning speed, interpretability)
  - Support for common and application-specific software development, technical research staff, establishing an interdisciplinary research community and close connection between the funding agencies and the research community