# QuantLab Virtual Workshop

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30th June 2021, Zürich

# Outline

1. **Computational graphs & deep learning frameworks**
   - Deep neural networks as computational graphs
   - Dynamic vs. static computational graphs
2. **QuantLab & `quantlib`**
   - The deep learning development stack
   - QNNs: a HW/SW co-design problem
3. **Graph editing**
   - Tree traversal and leaf replacement
   - Graph morphisms and algebraic graph rewriting

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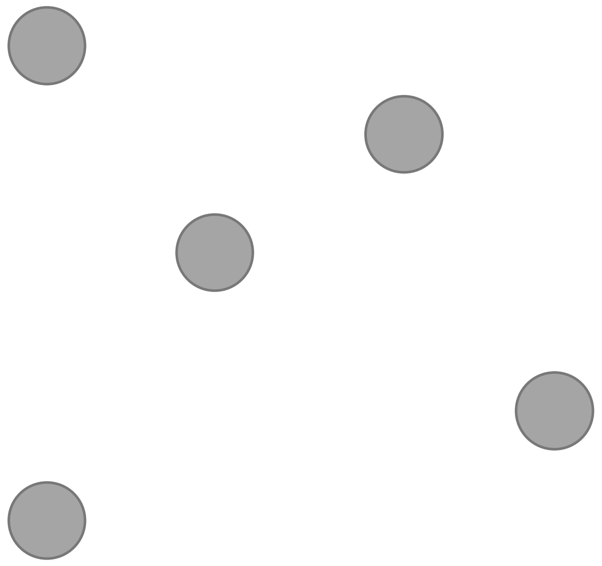
Part 1: computational graphs & deep learning frameworks

# Graph terminology - basics

- Let $V \neq \emptyset$ be a set of **nodes**



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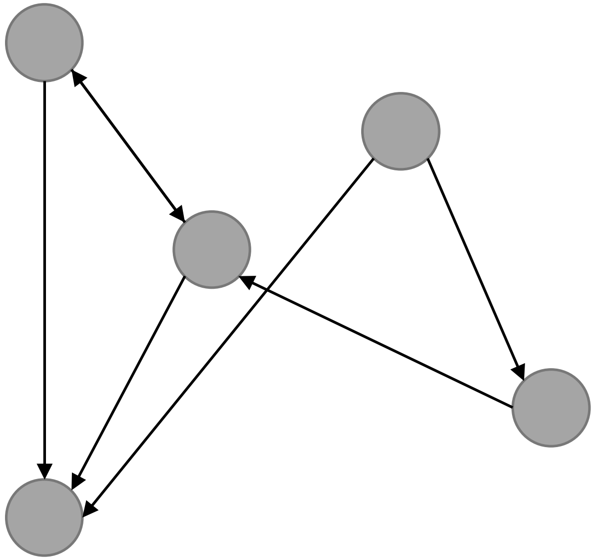

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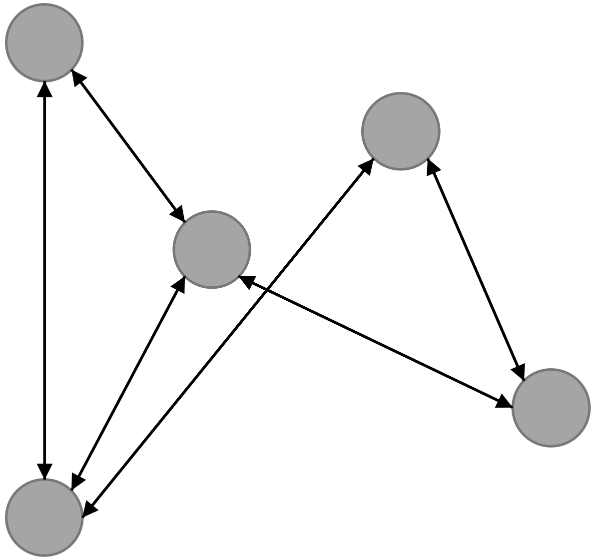

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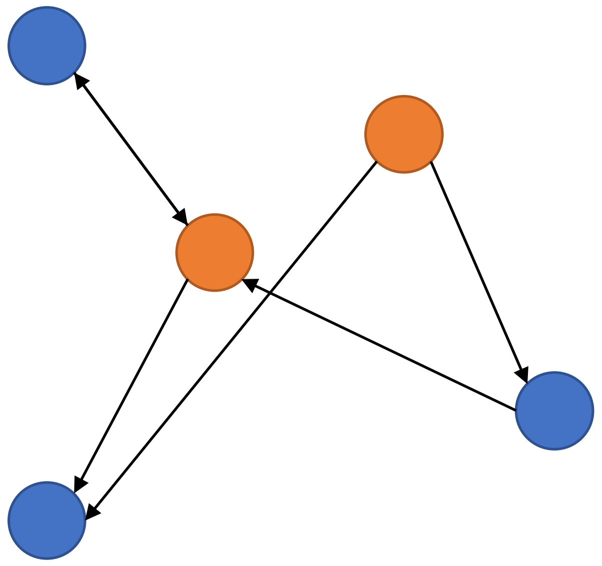
- **Bipartite graph**
  - $V = V_A \cup V_B \mid V_A, V_B \neq \emptyset, V_A \cap V_B = \emptyset$
  - $E \subseteq ((V_A \times V_B) \cup (V_B \times V_A))$



# Supervised learning: the problem

- The task is approximating an (unknown) function

$$f^* : X \to Y$$

- How can we assess the quality of an approximation $f \approx f^*$?
  - **Loss function**:

$$\ell : Y \times Y \to \mathbb{R}_0^+$$

  - **Loss functional**:

$$\mathcal{L}(f) \coloneqq \int_{X \times Y} \ell(f(x), y)\, d\mu(x, y)$$

# Supervised learning: the solution

- Machine learning system
  - **Hypothesis space**
    - $f : \Theta \times X \to Y$ (i.e., a collection $\{f_\theta : X \to Y \mid \theta \in \Theta\}$)
    - Rewrite $\mathcal{L}(f) = \mathcal{L}(\theta) = \int_{X \times Y} \ell(f(\theta, x), y) d\mu(x, y)$
  - **Data set**
    - $\mathcal{D} : X \times Y \to \mathbb{N}_0 \mid 0 < \sum_{(x,y) \in X \times Y} \mathcal{D}(x, y) = N < +\infty$
    - Approximate $\mu \approx \frac{1}{N} \sum_{(x,y) \in X \times Y} \mathcal{D}(x, y) \delta_{(x,y)}$
  - **Learning algorithm**
    - If $\mathcal{L}$ and $f$ are differentiable, it can be gradient-based:

$$\theta_{t+1} = \theta_t - \eta \nabla_\theta \mathcal{L}(\theta_t) = \theta_t - \eta \left(\frac{1}{N} \sum_{(x,y) \in X \times Y} \mathcal{D}(x, y) \nabla_\theta \ell(f(\theta_t, x), y)\right)$$

# Computational graphs

- Directed, bipartite graphs
- $V = V_M \cup V_K$
  - *Memory nodes* $v \in V_M$ represent operands
  - *Kernel nodes* $v \in V_K$ represent operations
- $E \subseteq ((V_M \times V_K) \cup (V_K \times V_M))$
  - Arcs $e \in E \cap (V_M \times V_K)$ represent *read/load* dependencies
  - Arcs $e \in E \cap (V_K \times V_M)$ represent *write/store* dependencies
- Each operand is the result of at most one operation:
  - $\forall v \in V_M, (u_1, v), (u_2, v) \in E \Rightarrow u_1 = u_2$

# DNNs as computational graphs: an example

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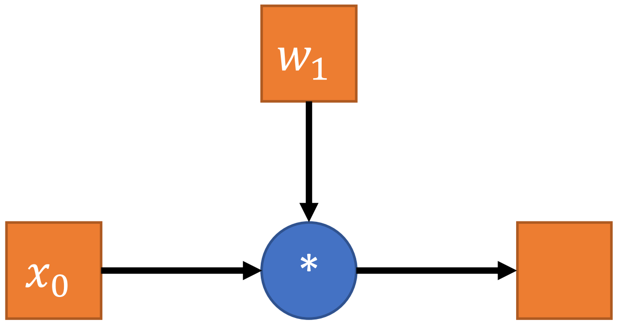

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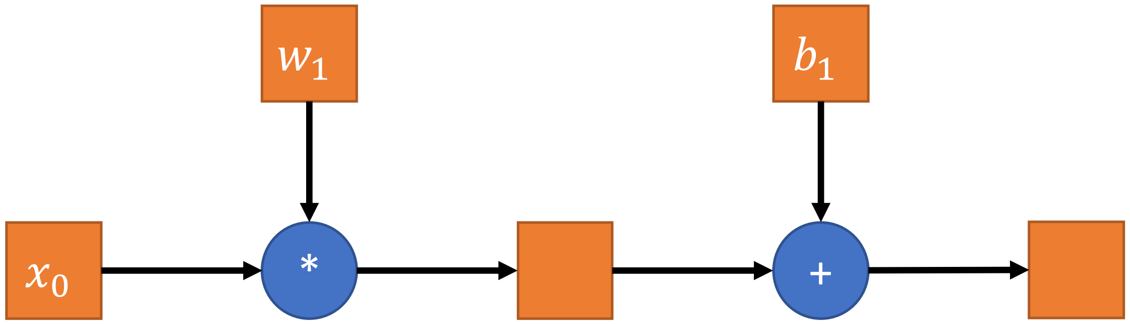

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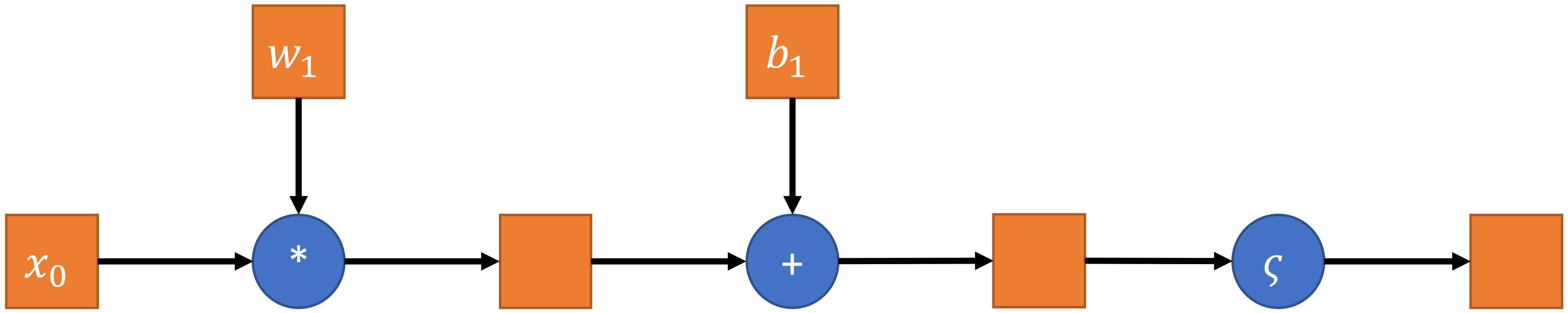

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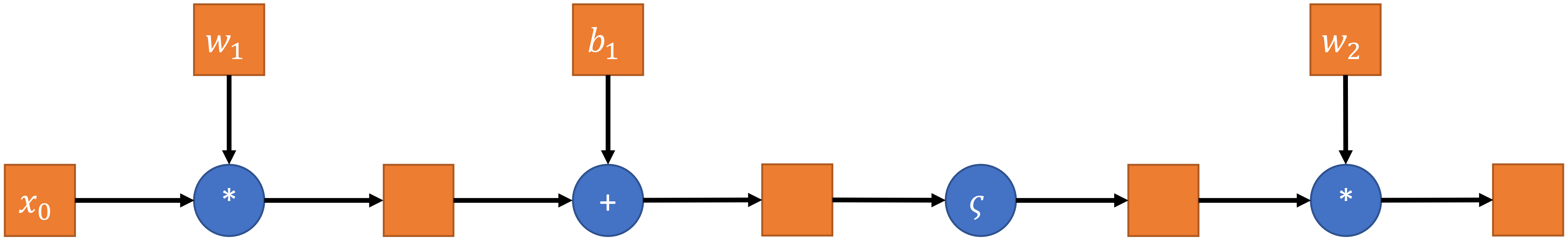

# Three ways of performing differentiation

- Symbolic differentiation
  - Based on the rules of differential calculus
  - Given a function $\mathcal{L}(\theta, z)$, *pre-compute* $\nabla_\theta \mathcal{L}|_{\theta,\, z}$ as a function of $\theta$ and $z$.
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- Numerical differentiation
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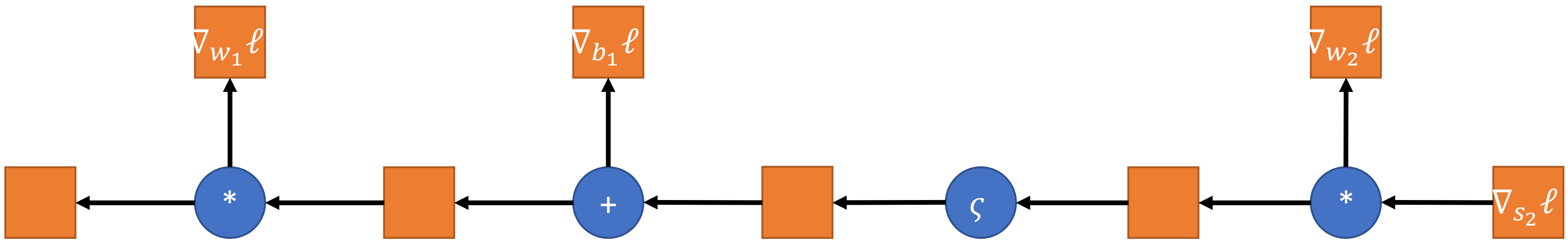
- **Automatic differentiation**

# Automatic differentiation

- Based on the chain rule
- Each operation computes the gradients with respect to its inputs
- Two modes
  - **Direct-mode**
    - Can be computed in parallel to the forward pass
    - Almost always **requires recomputing** tensor contractions
  - **Reverse-mode** (aka **back-propagation**)
    - Must wait the completion of the forward pass before beginning the gradient computation
    - **Computes each product** in the chain rule **just once**

# Differentiable computational graphs

- Each operation $v \in V_K$ is differentiable with respect to its operands $u \in V_M | \, (u, v) \in E$
- *Forward pass* (aka *inference pass*)
- *Backward pass*
  - This is gradient computation
  - Do **not** confuse it with gradient descent!



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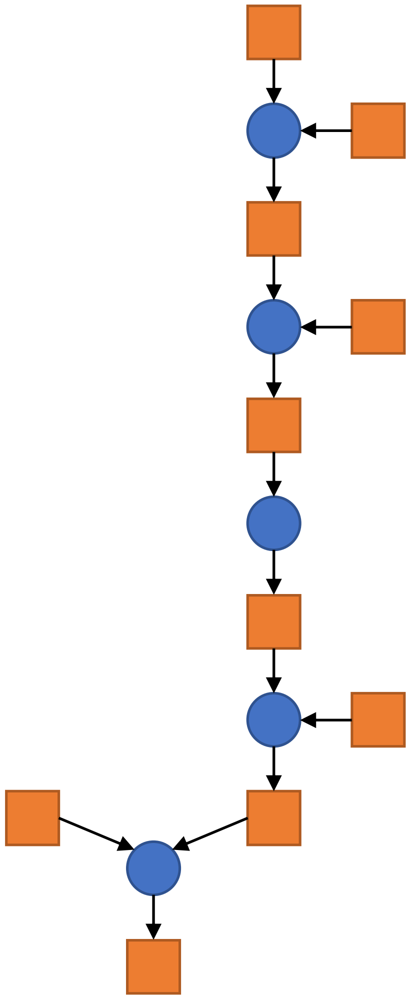

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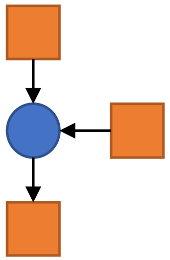

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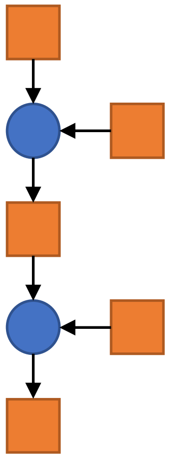

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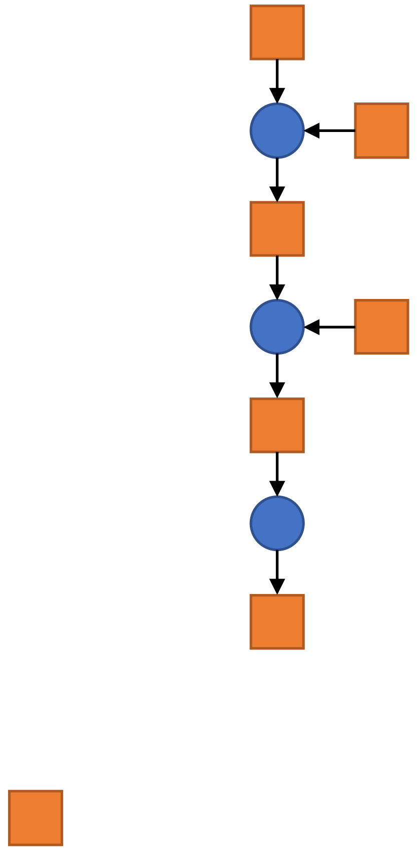

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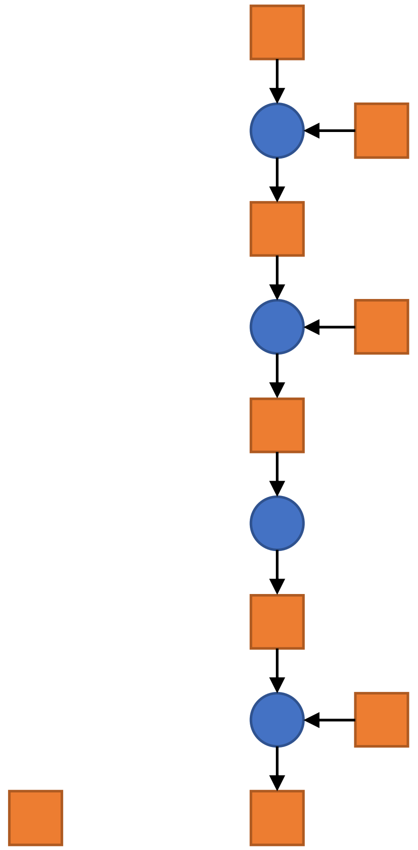

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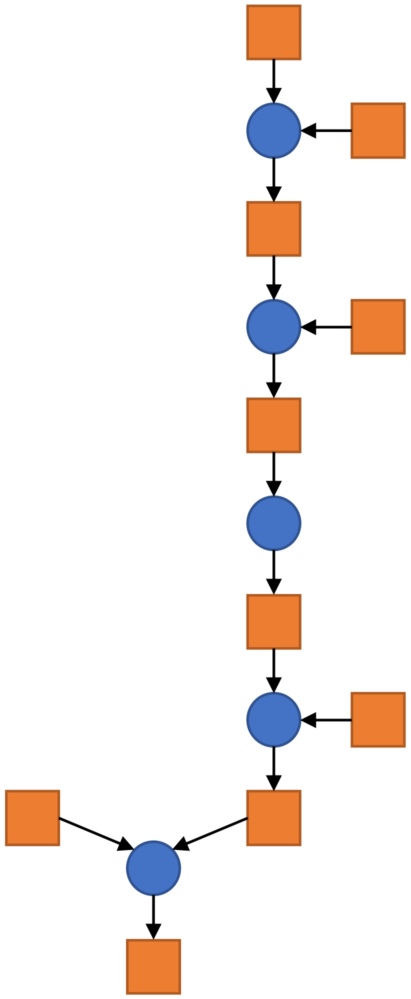

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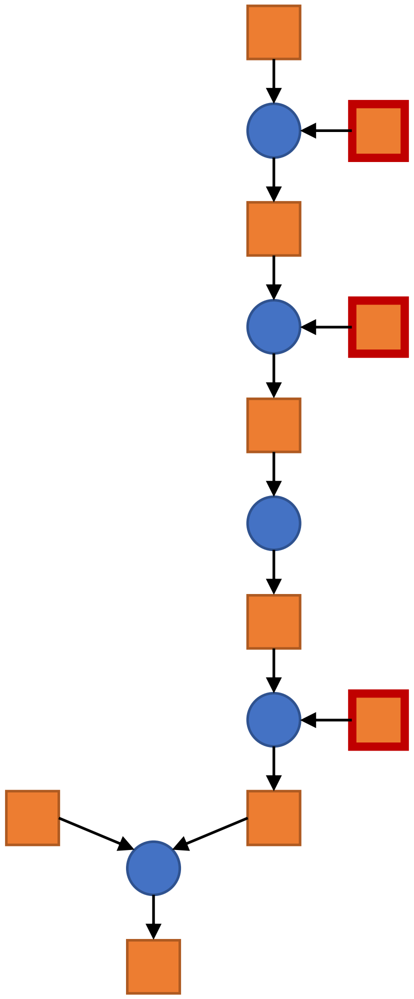

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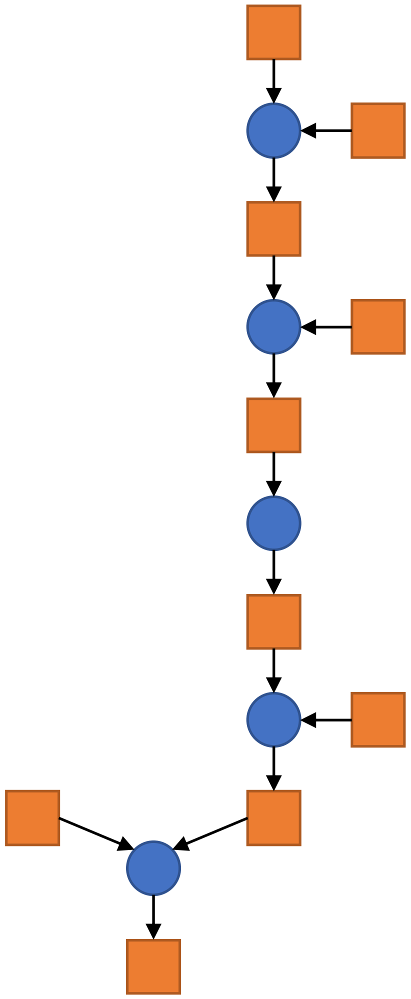

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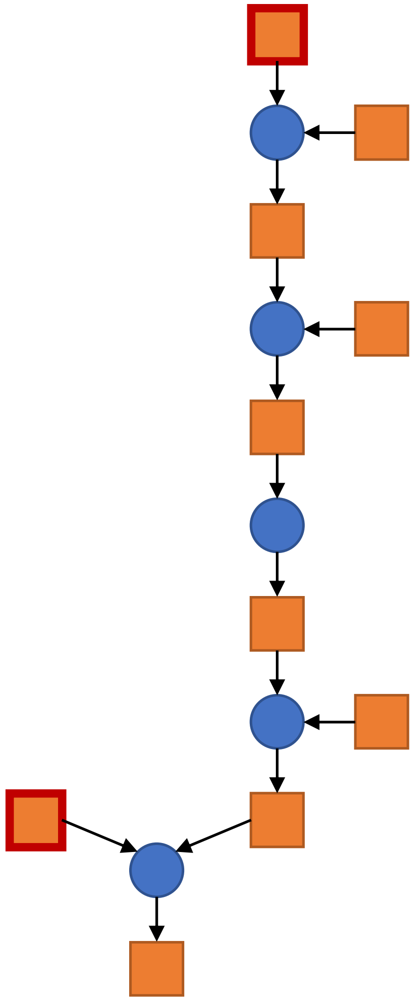

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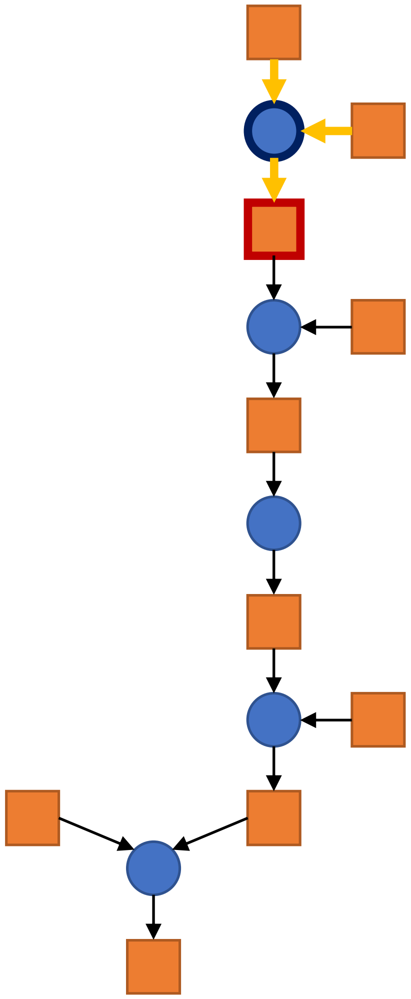

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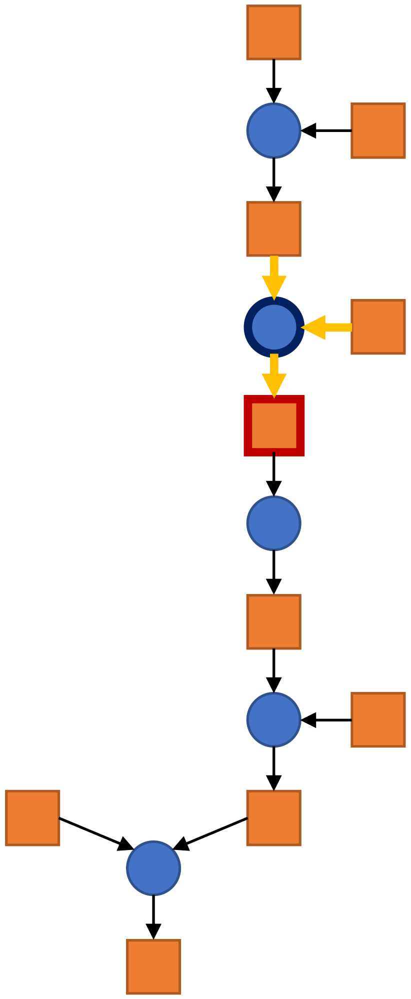

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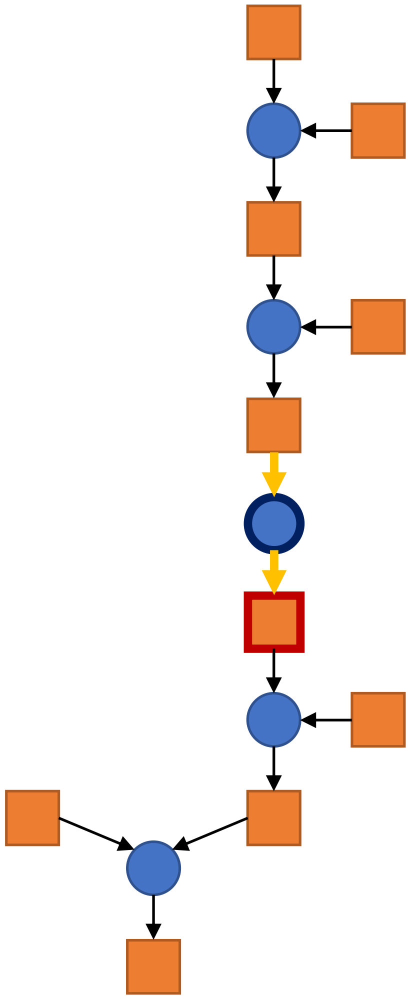

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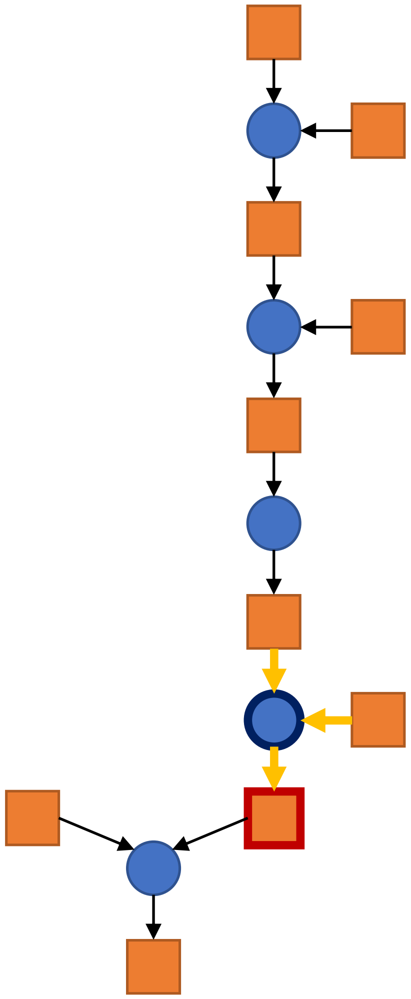

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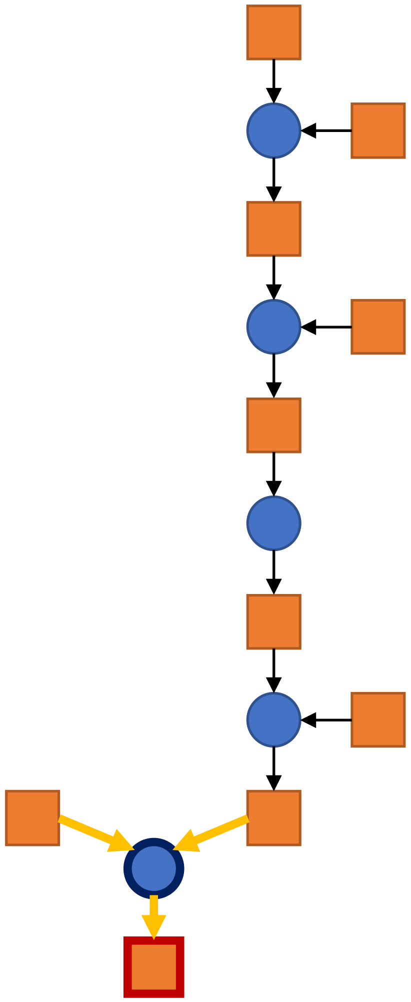

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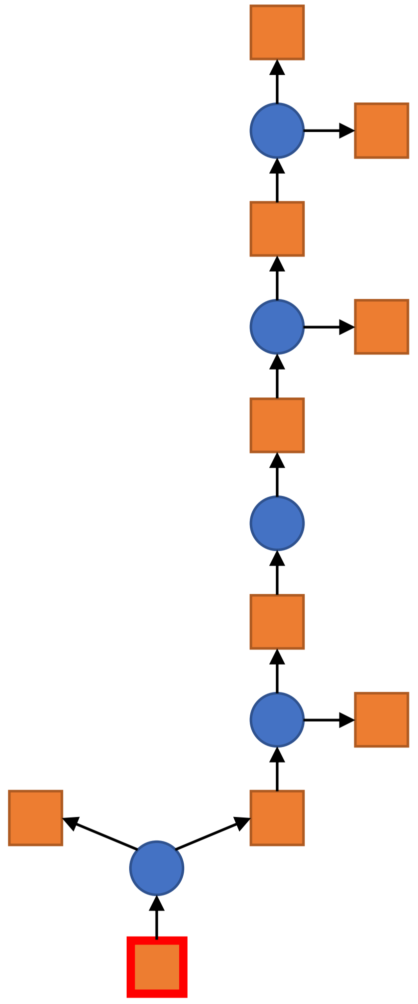

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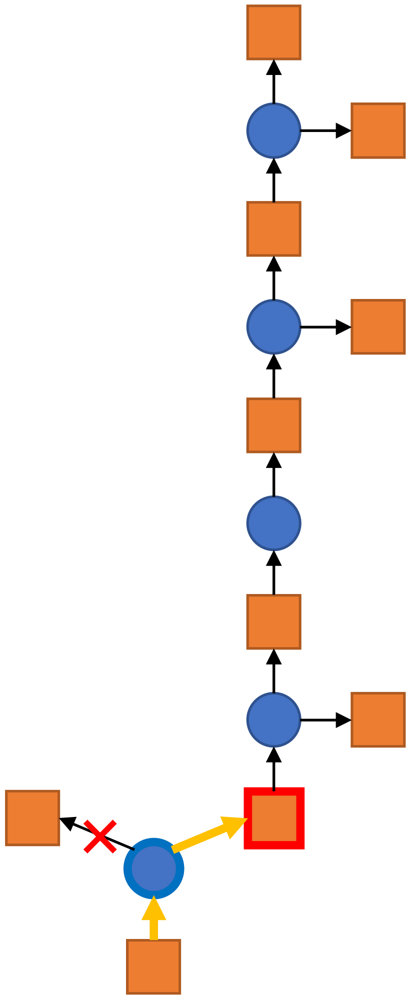

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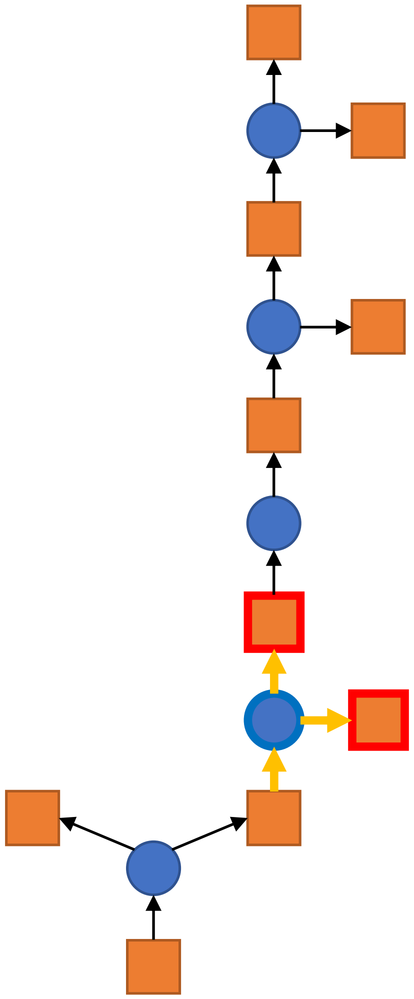

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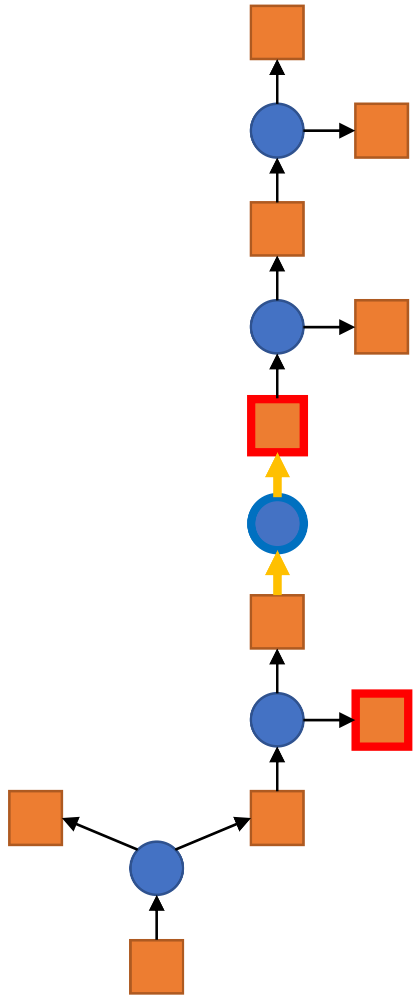

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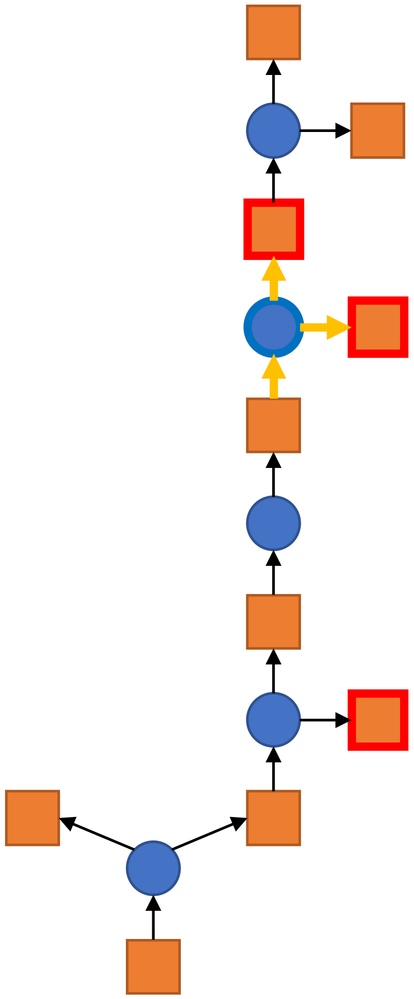

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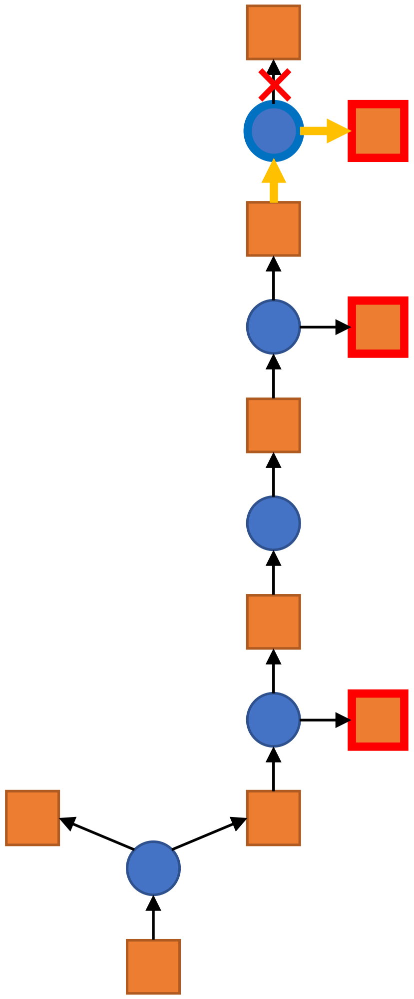

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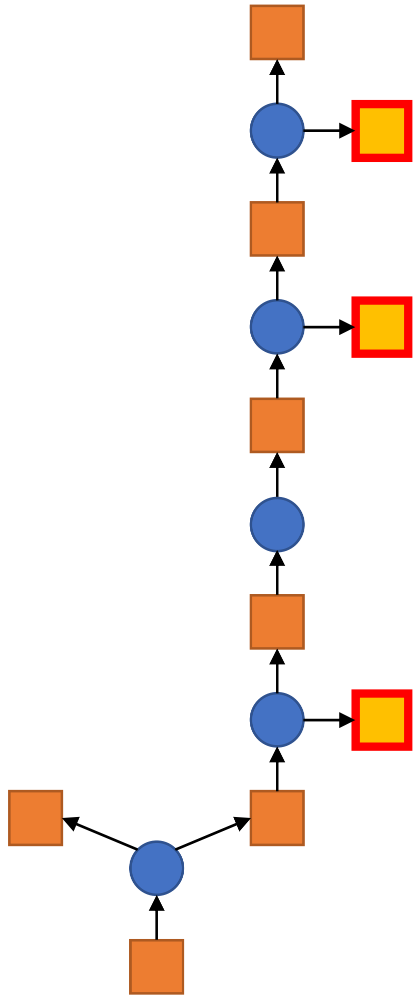

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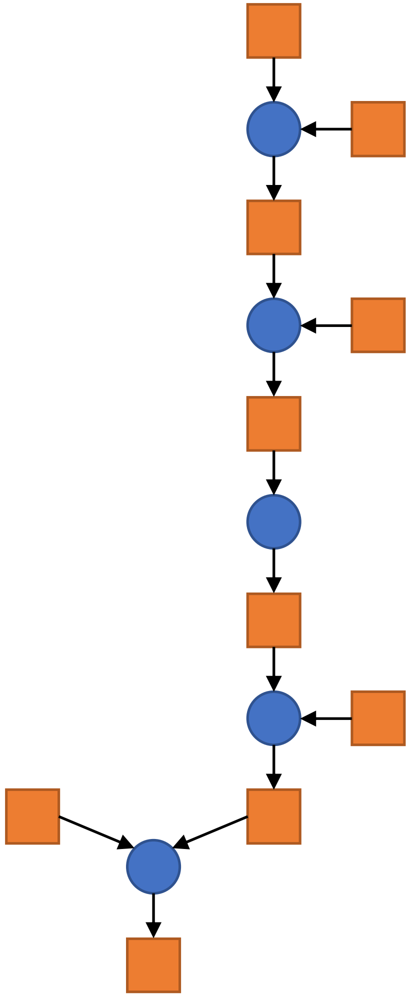

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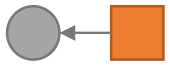

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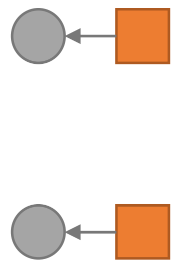

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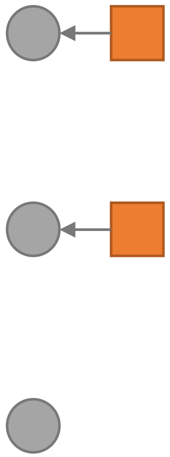

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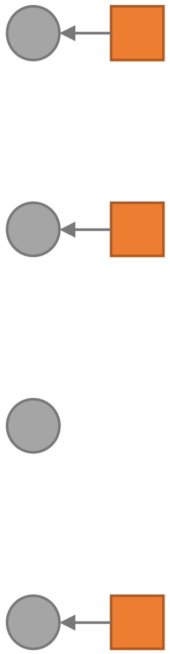

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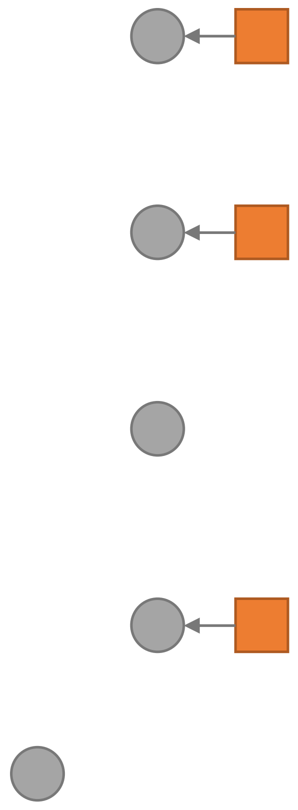

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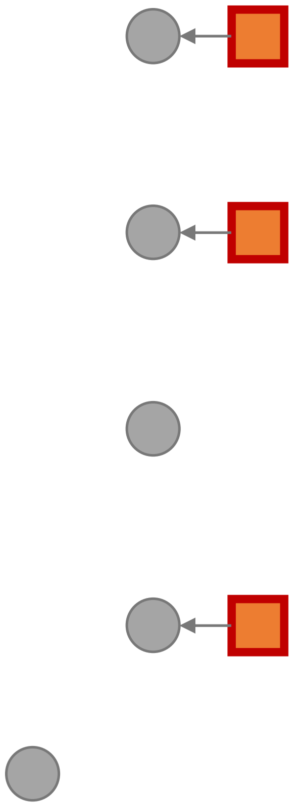

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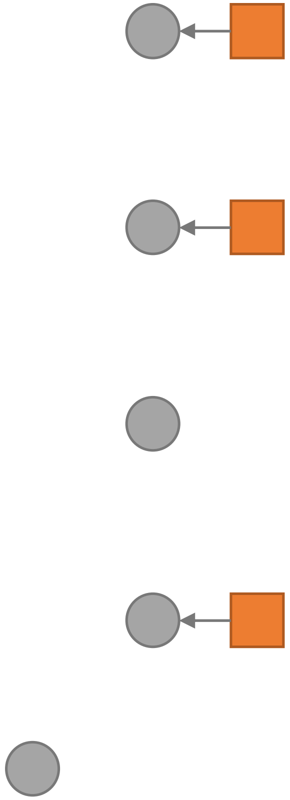

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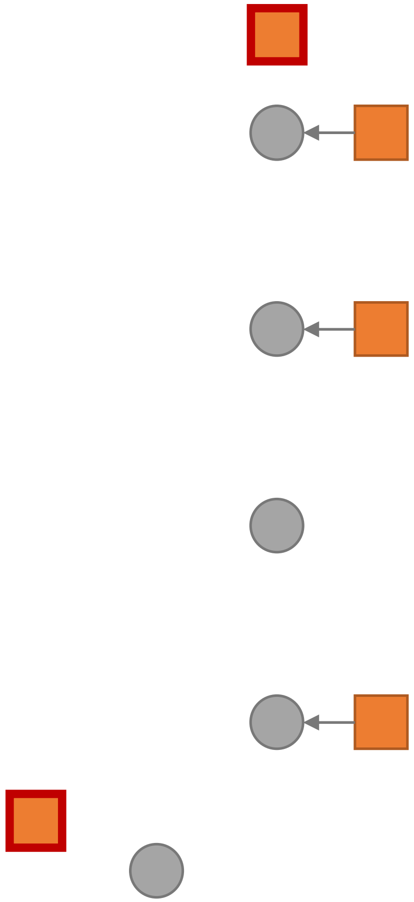

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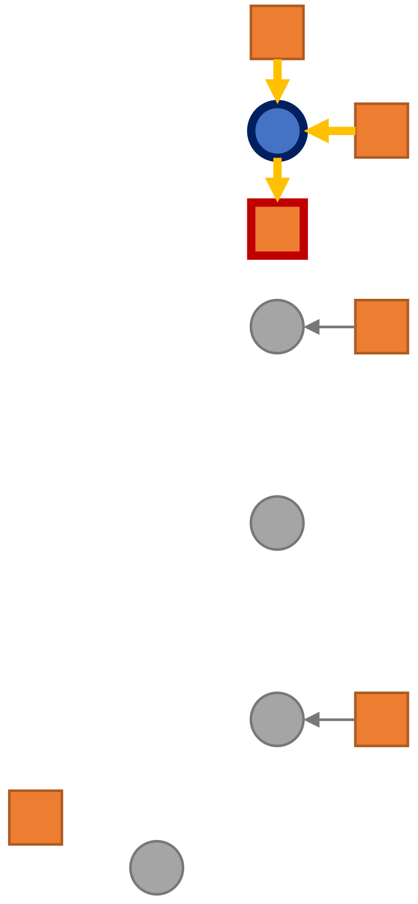

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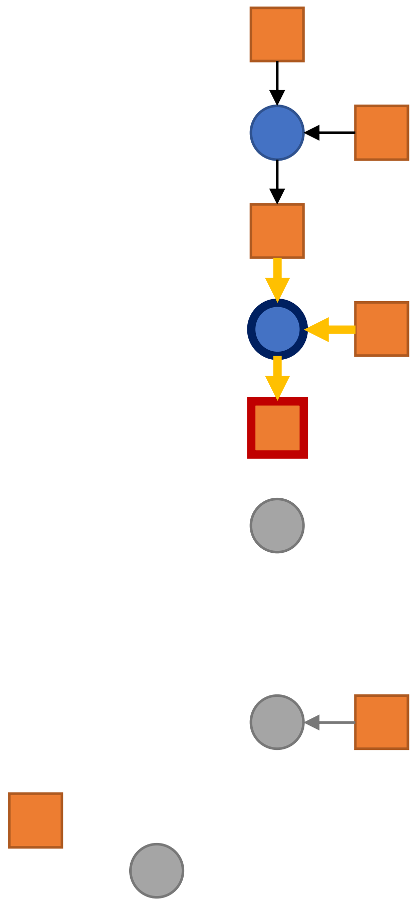

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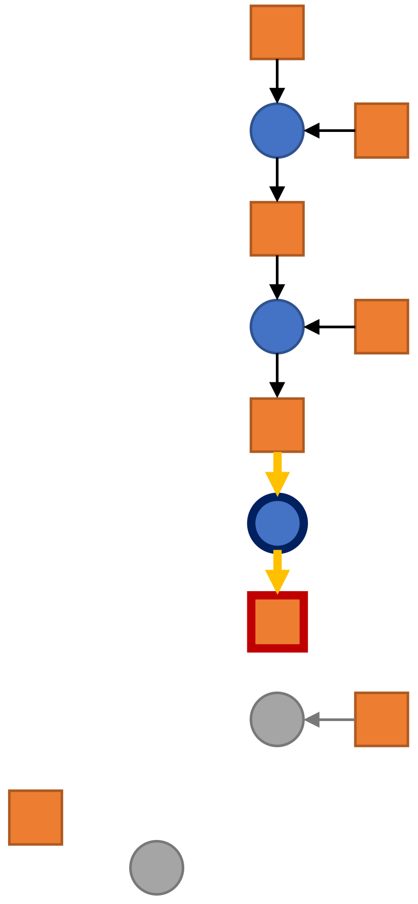

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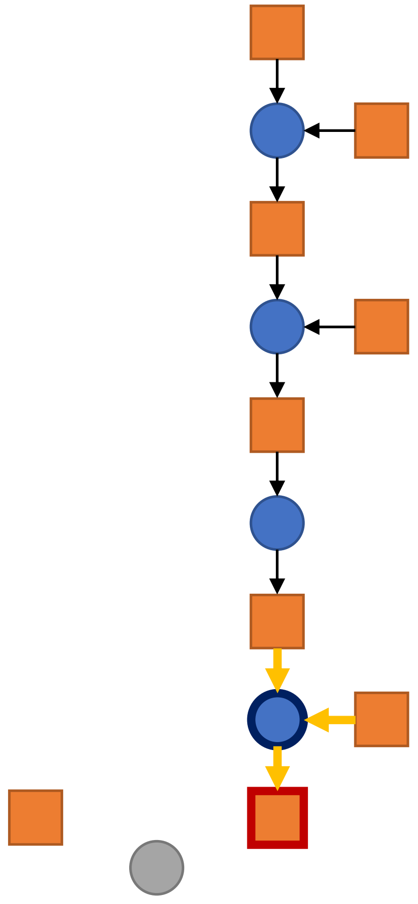

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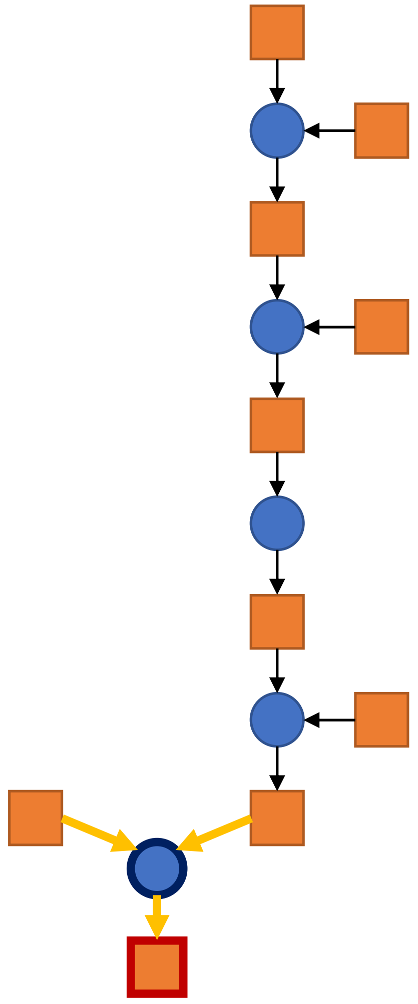

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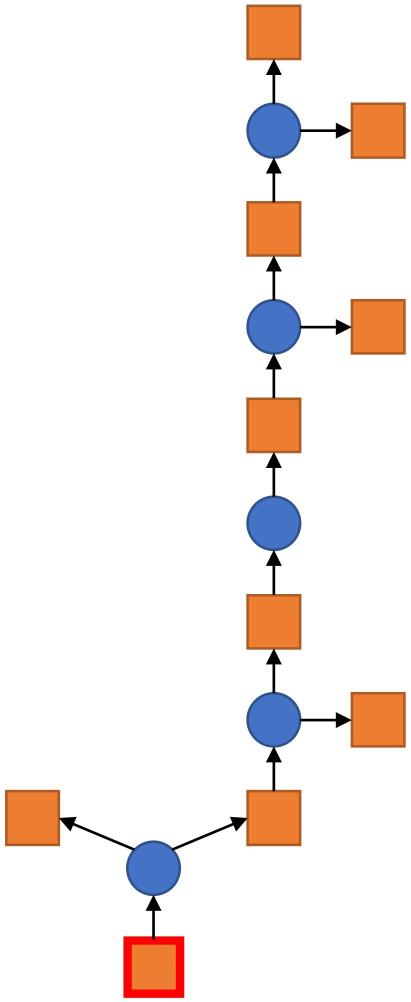

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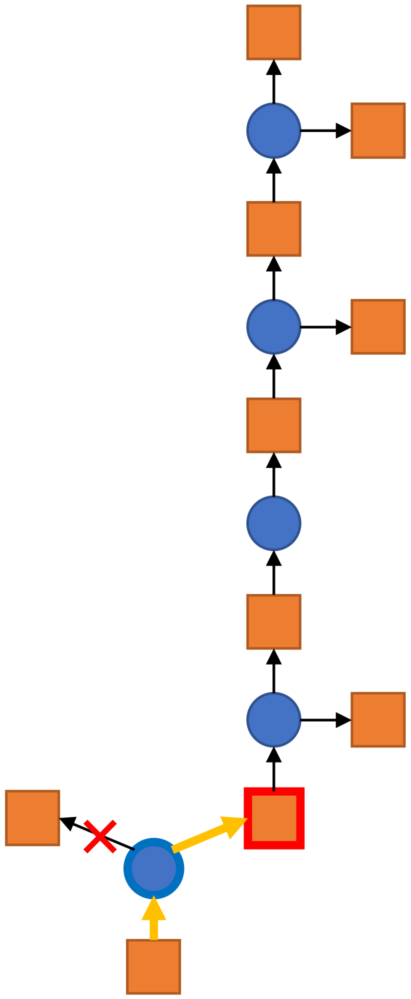

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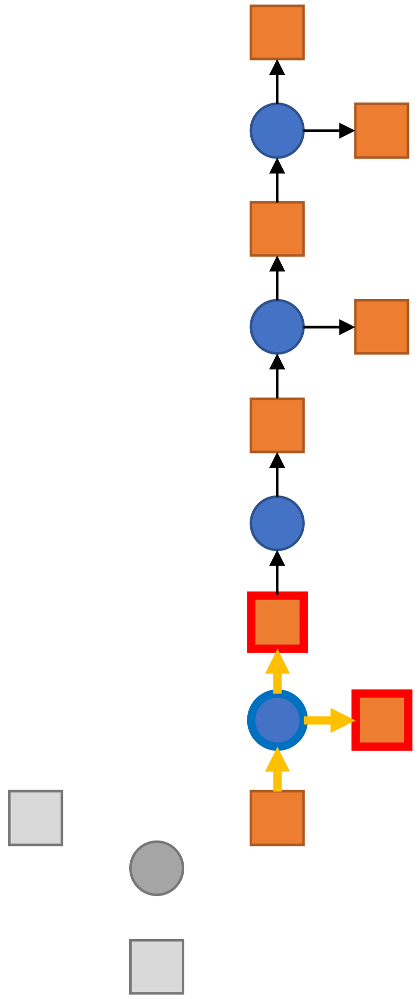

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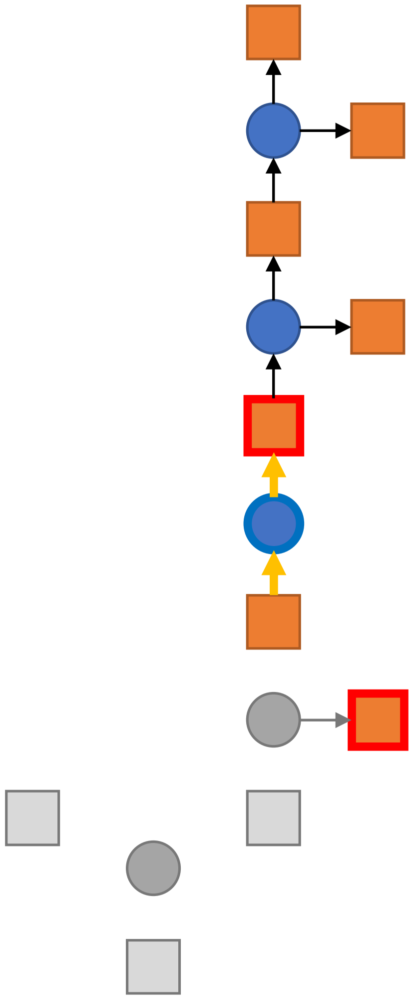

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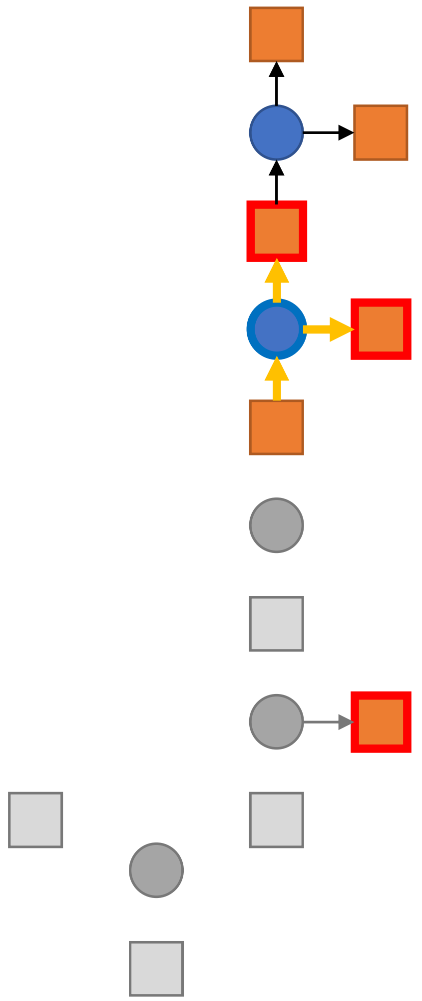

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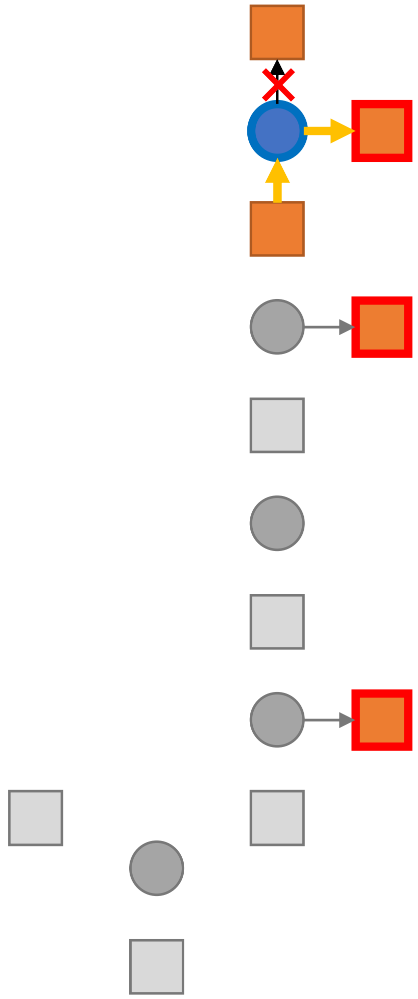

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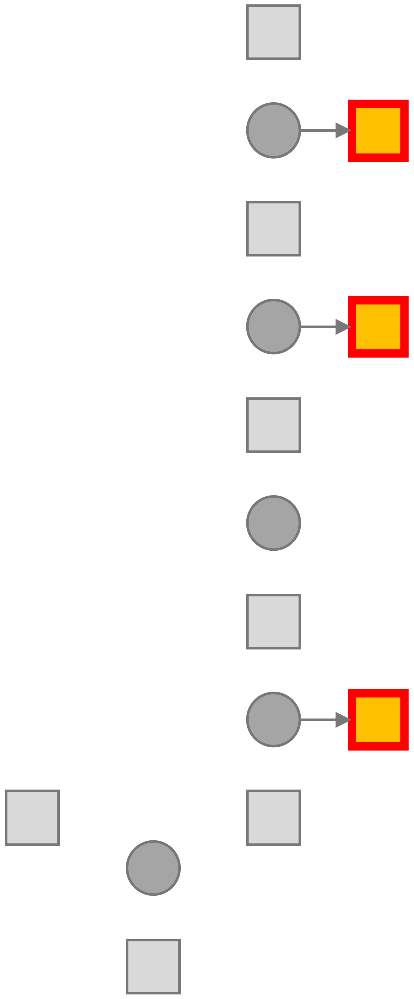

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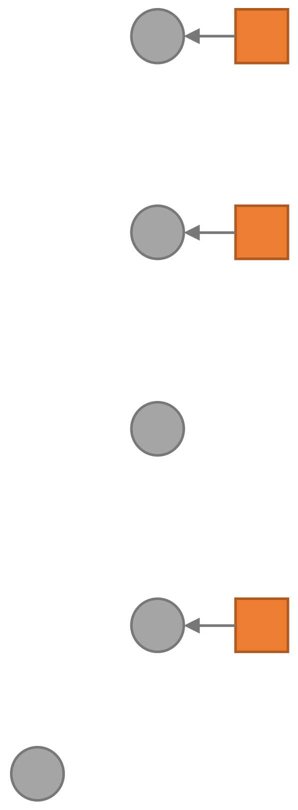
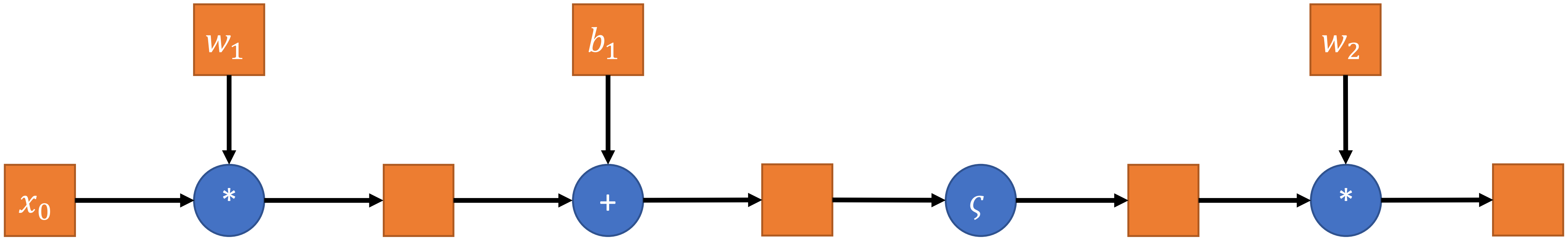


# A thousand flavours of computational graphs

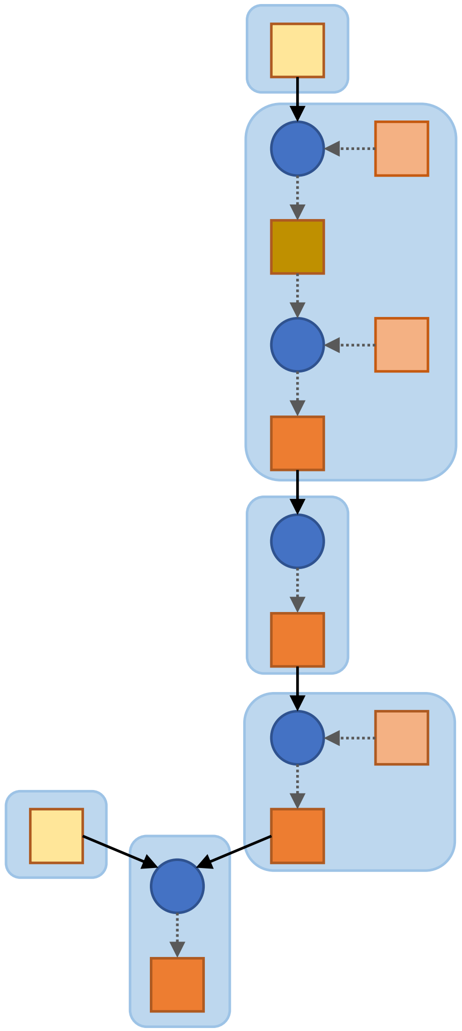
ONNX: the “assembly” of computational graphs



# A thousand flavours of computational graphs

TensorFlow (v1.0 – might have changed)

- Operation “super-nodes” contain:
  - Memory nodes
    - Constants
    - Parameters
    - Hyper-parameters
    - Output features
  - Kernel nodes
- Edges can be associated to the output memory nodes contained in each “super-node”
  - “Nodes represent operations, edges represent data flowing between operations”



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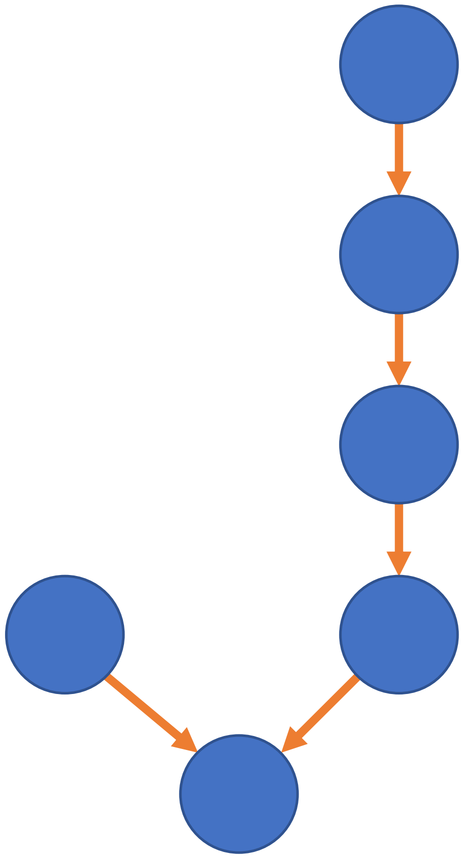

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PyTorch (v1.9)

- Operation "super-nodes" contain:
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    - Defined <u>explicitly</u> in the constructor (`__init__`) method
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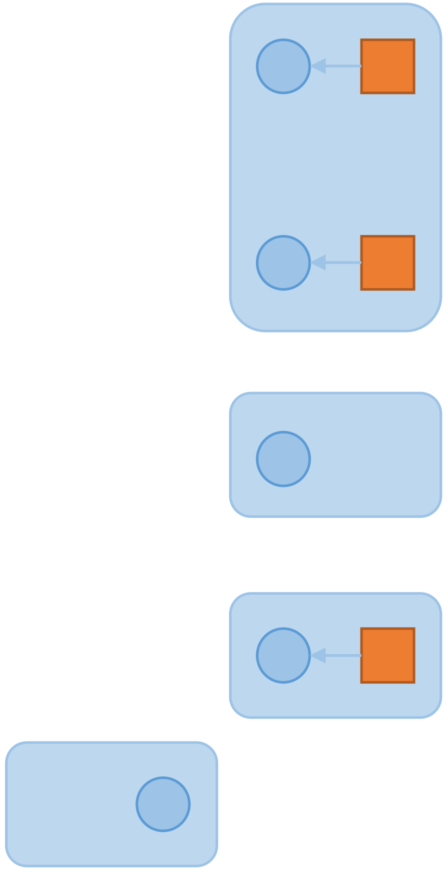

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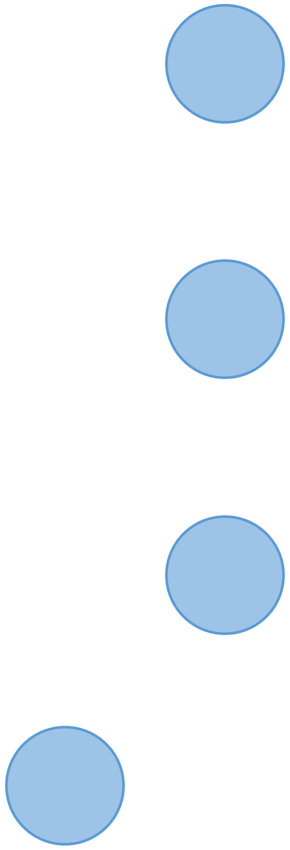

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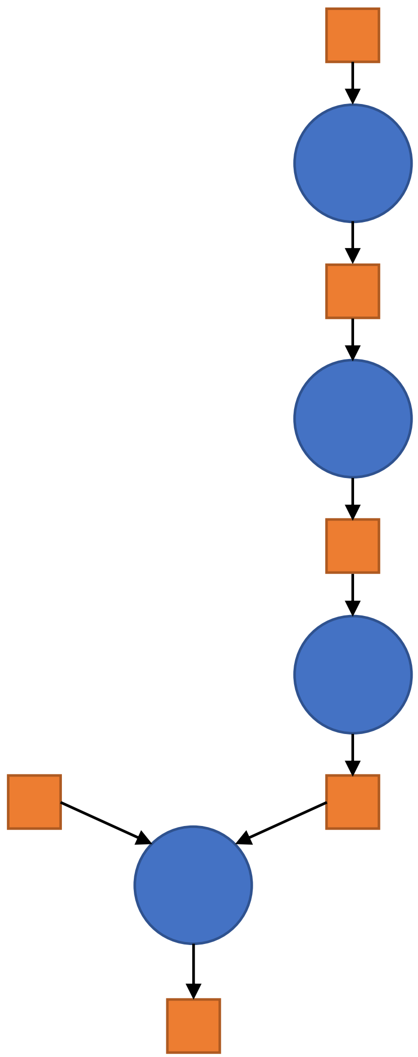
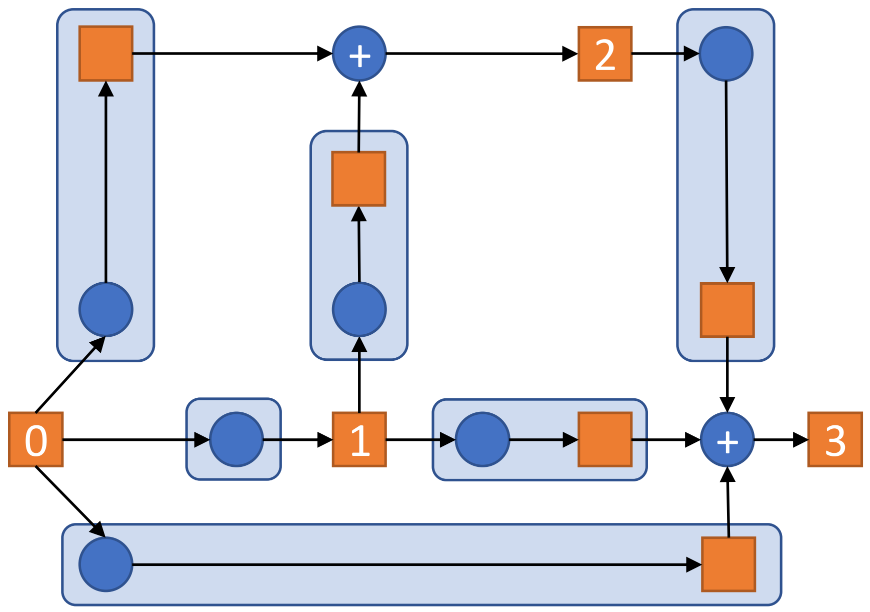


# A thousand flavours of computational graphs

NASBench201 data set

- *Neural architecture search* (NAS) is a deep-learning-specific variant of *model selection*
- NASBench201
  - Inputs: *genotypes*, i.e., structured description of network topologies
  - Outputs: accuracies
- Genotypes are described in terms of cells
  - Nodes represent feature arrays
  - Edges represent operations and their parameters



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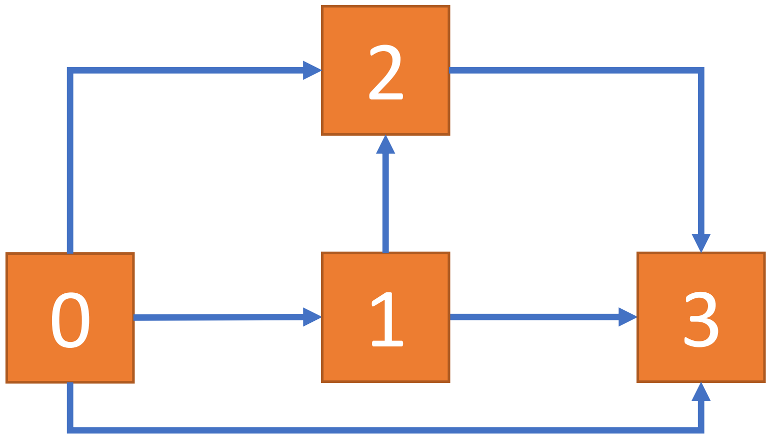
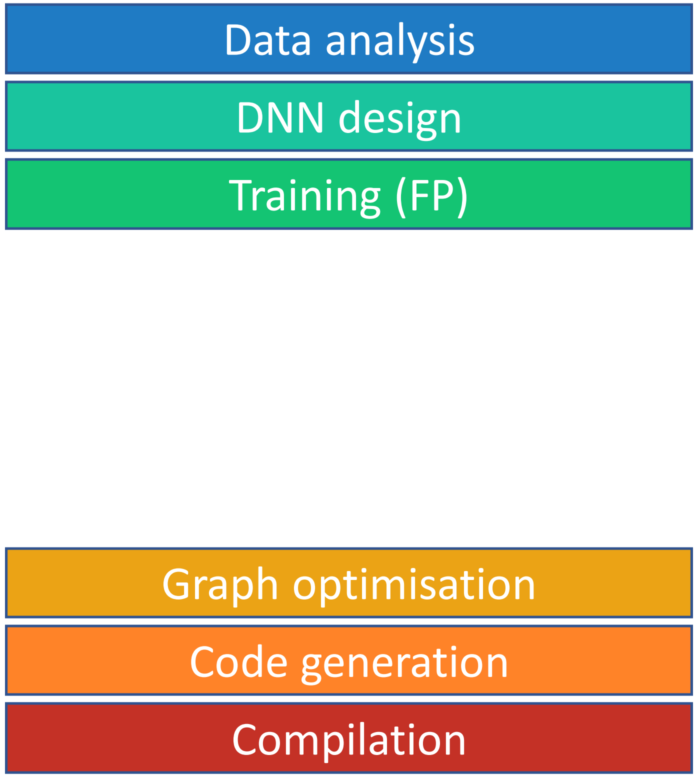


# QuantLab Virtual Workshop

Part 2: QuantLab & `quantlib`

# The deep learning development stack



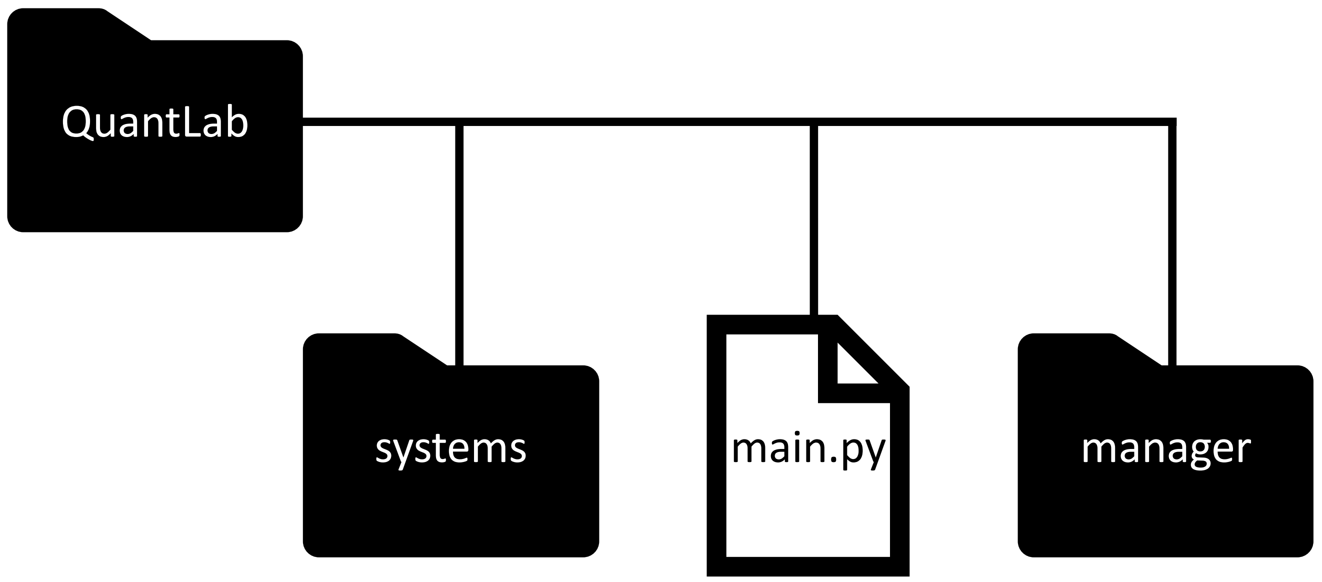

**Platform-agnostic**

- **Data analysis**: how can we model the data problem?
- **DNN design**: which network topology can work best?
- **Training**: backpropagation + SGD

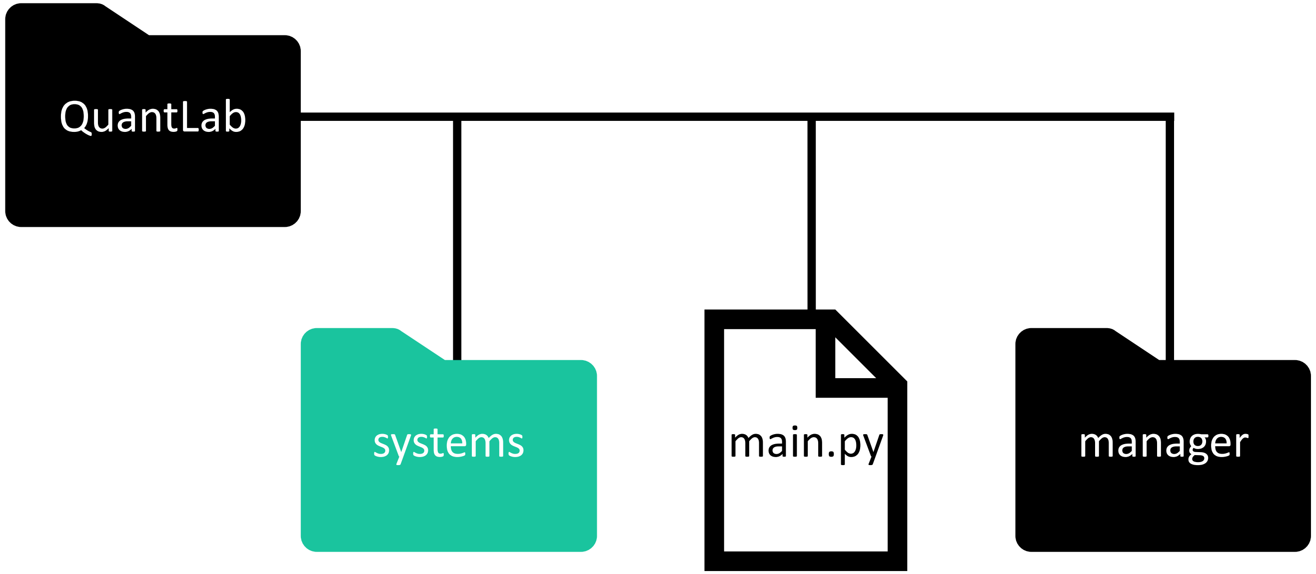
**Platform-specific**

- **Graph optimisation**: ONNX graph (e.g., tiling, “node fusion”)
- **Code generation**: from ONNX graph to C/C++ code
- **Compilation**: from C/C++ code to machine code

# QuantLab: structure overview



# QuantLab: the `systems` package



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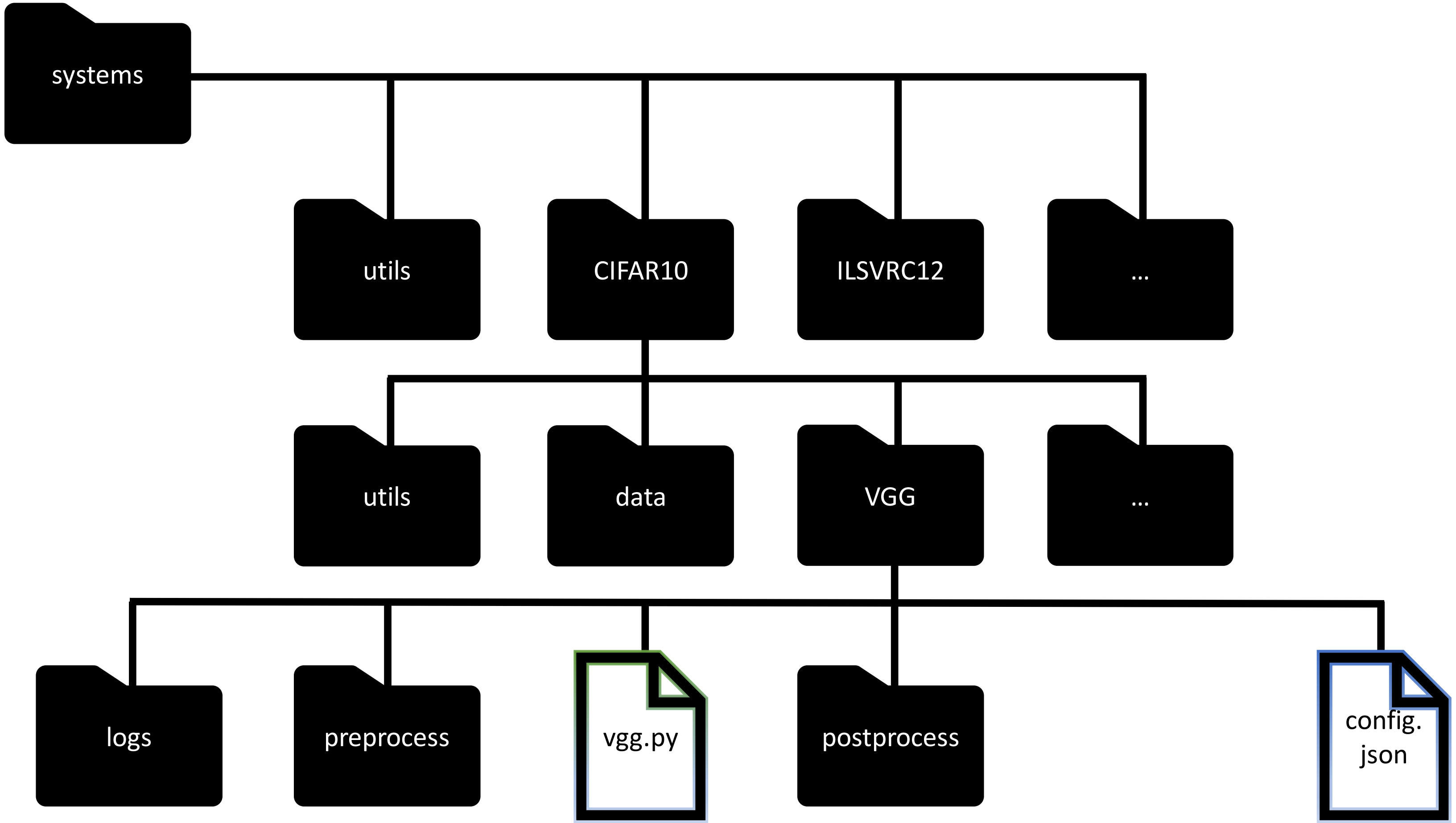

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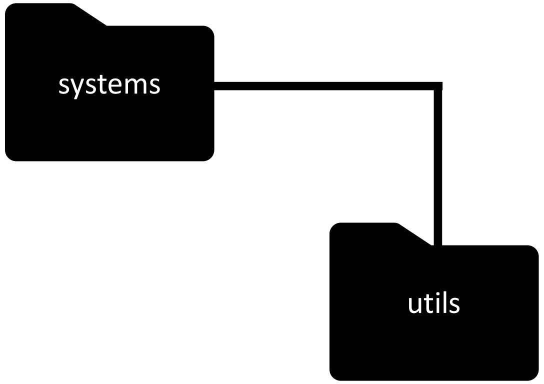
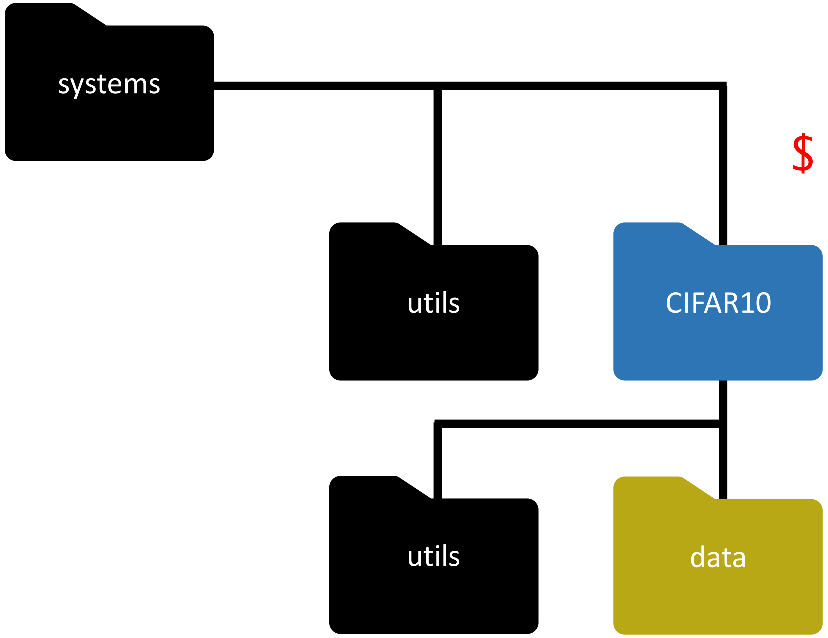
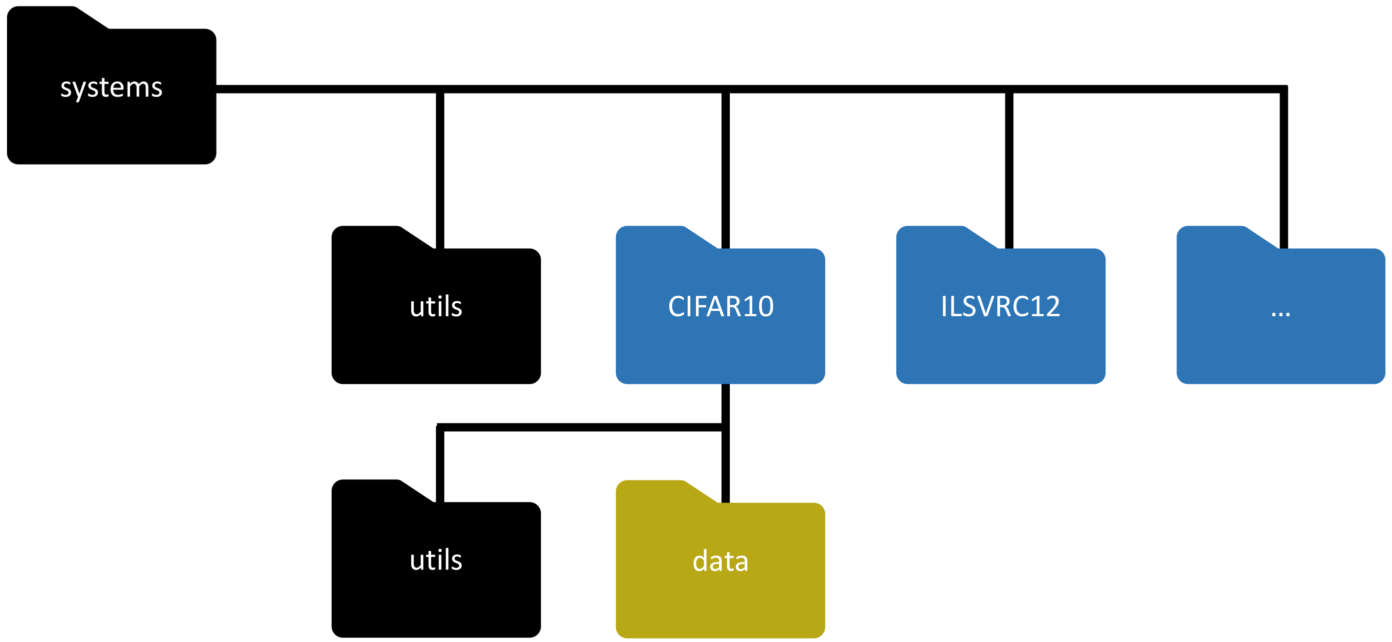


# The `systems` package: problem sub-package

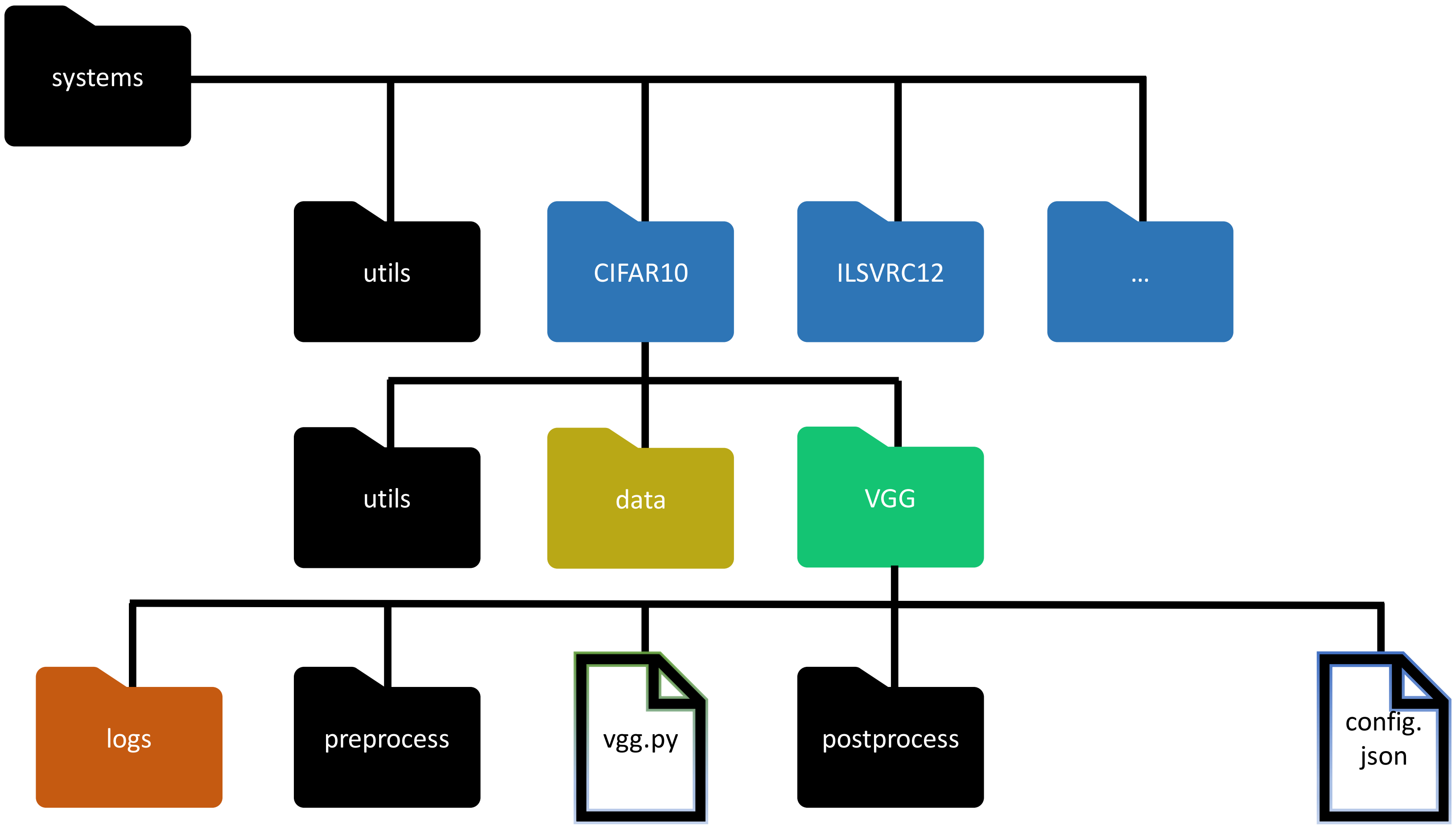



```
$ bash configure/problem.sh CIFAR10
```

# The `systems` package: adding problems



# The `systems` package: topology sub-package

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$ bash configure/problem.sh CIFAR10 VGG
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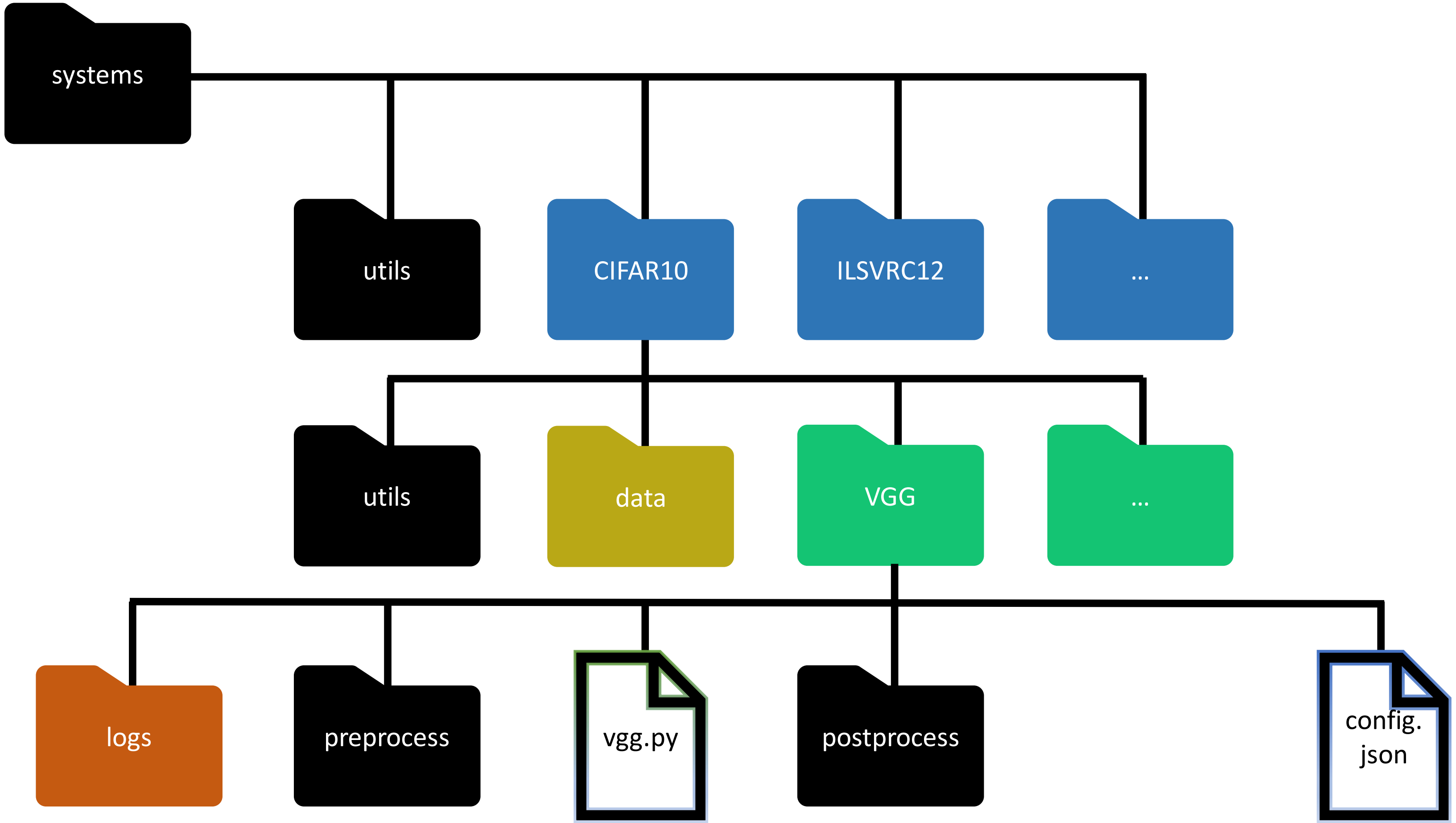

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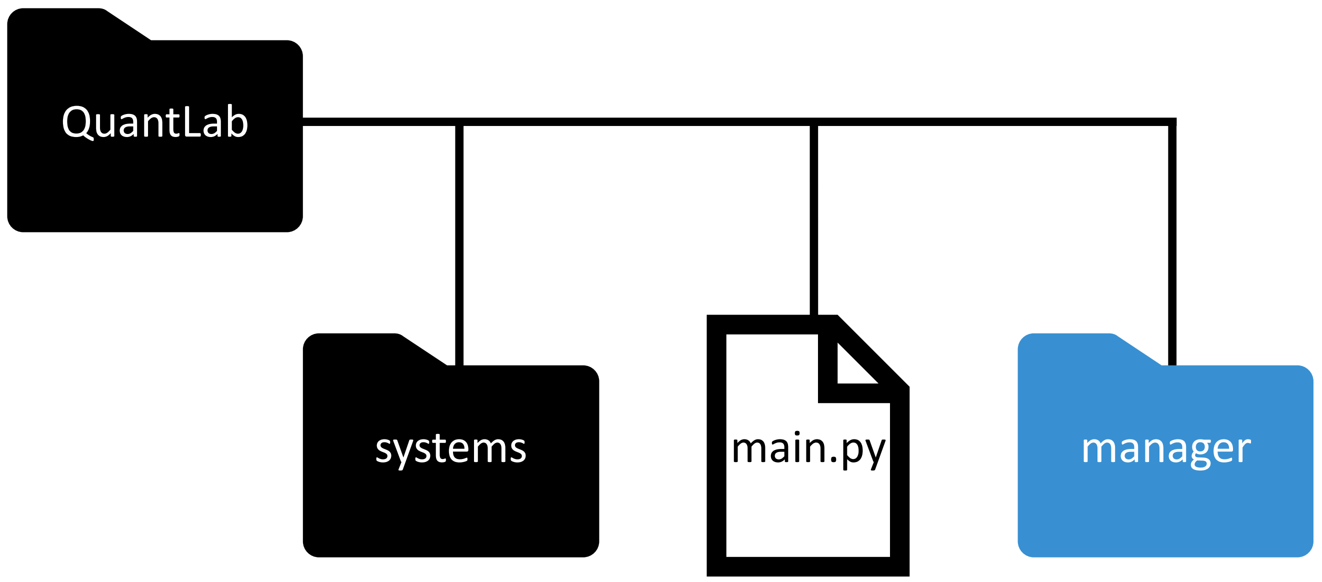

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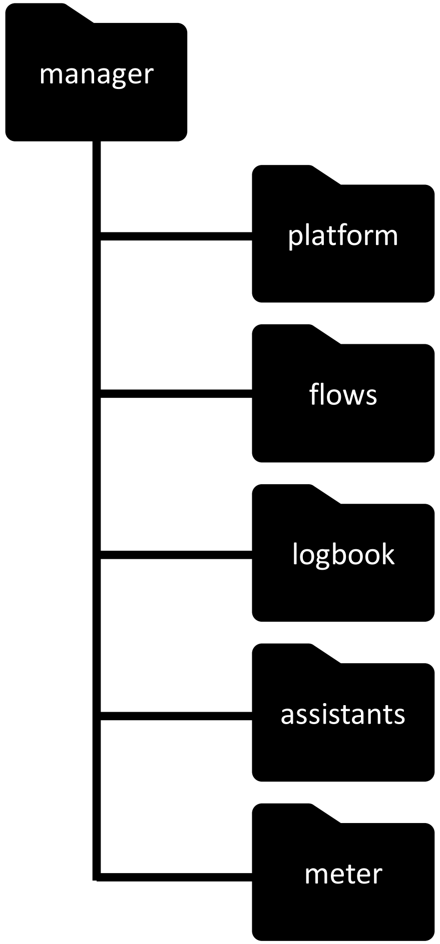
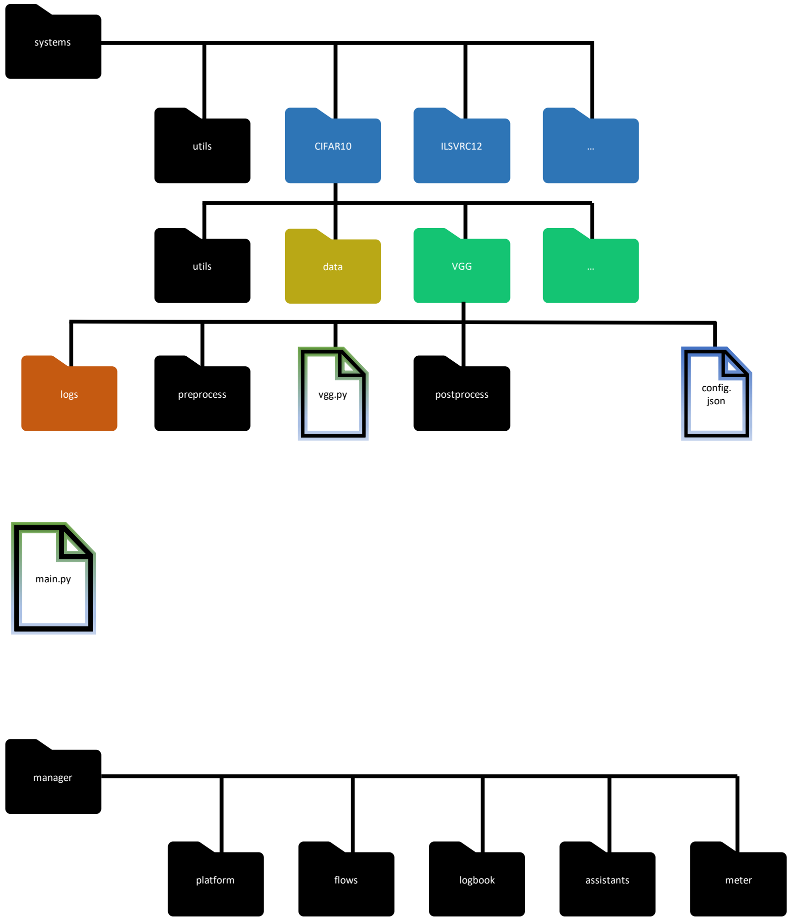
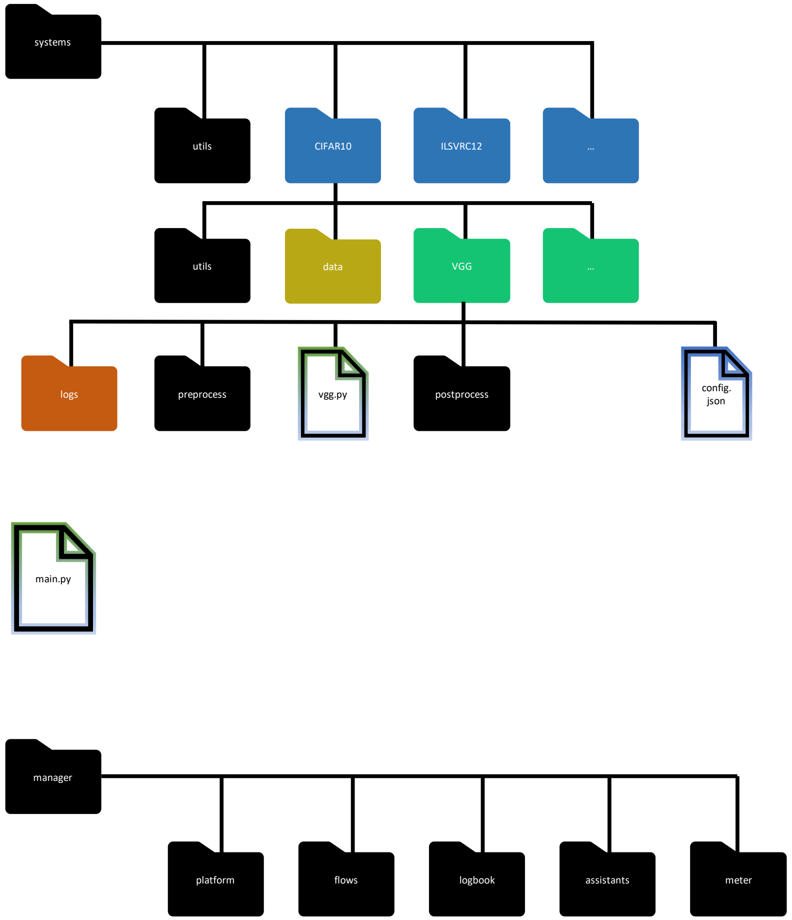



- **`platform`**: management of HW/OS aspects (e.g., GPU aspects, distributed processing)
- **`flows`**: the services that can be accessed from the façade
- **`logbook`**: the abstraction that mediates the interactions between the QuantLab flows and the disk
- **`assistants`**: the abstractions that assemble the components of the deep learning systems inside QuantLab flows
- **`meter`**: the abstractions to track statistics on parameters and features of the deep neural network being trained or tested

# QuantLab *flows*



# QuantLab *flows*: configuring an experiment




$ python main.py –problem=CIFAR10 –topology=VGG configure

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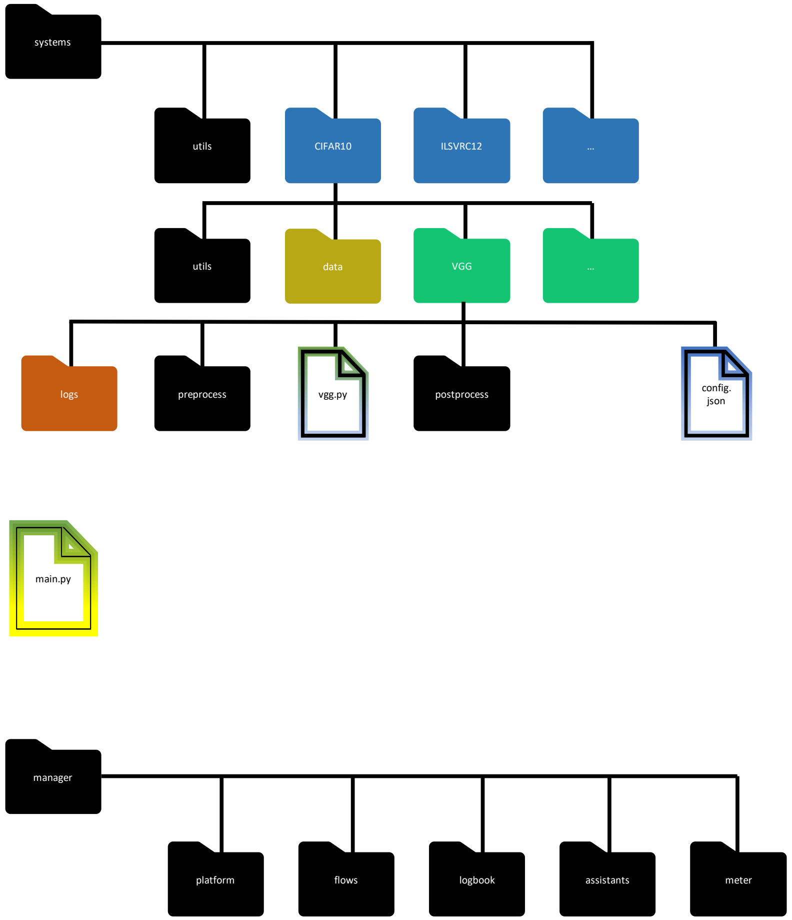


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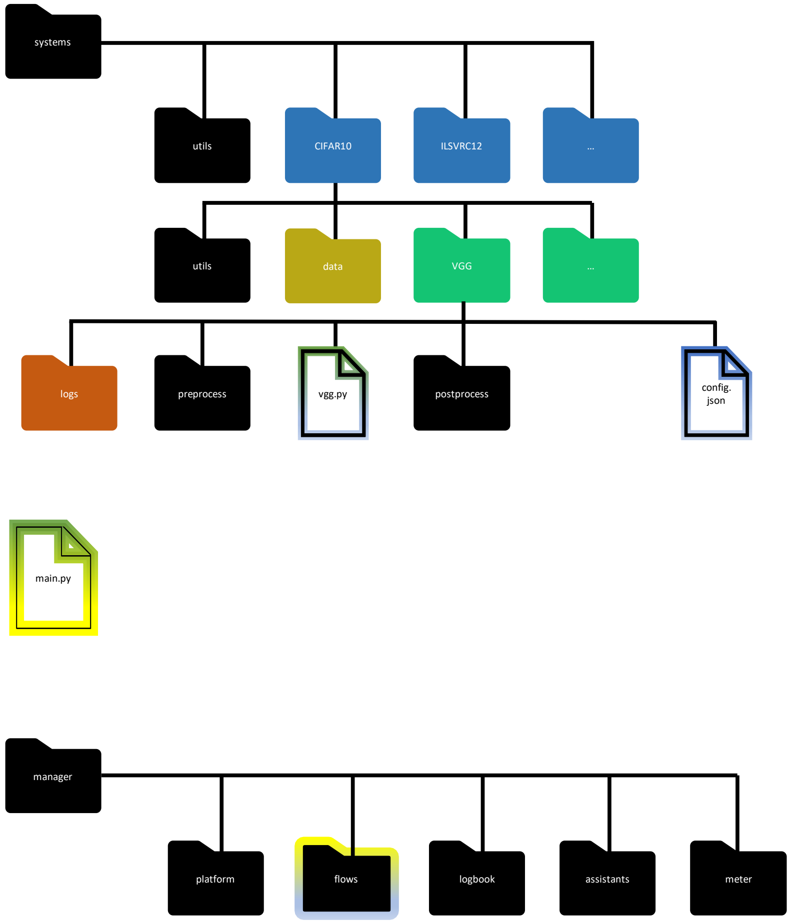


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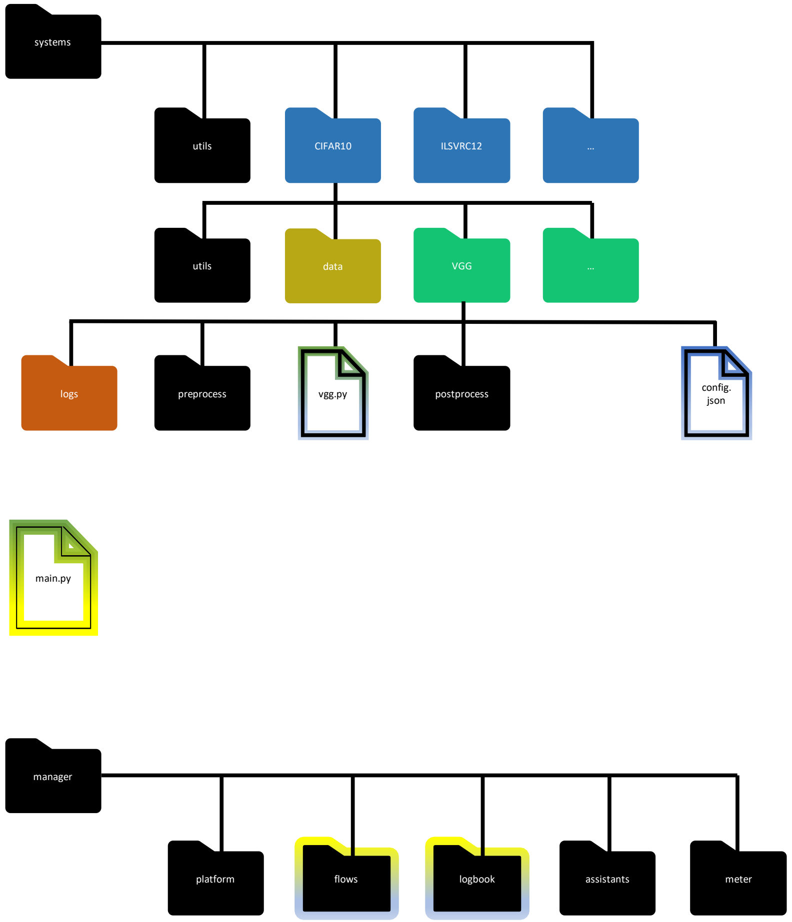


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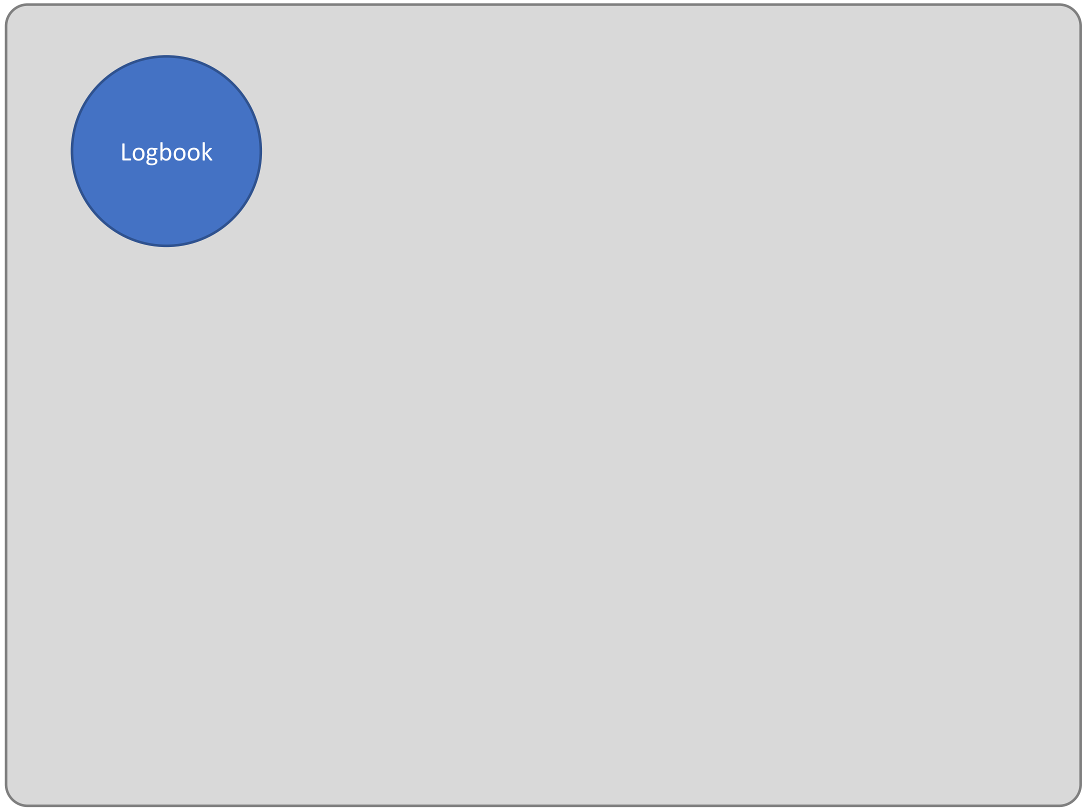

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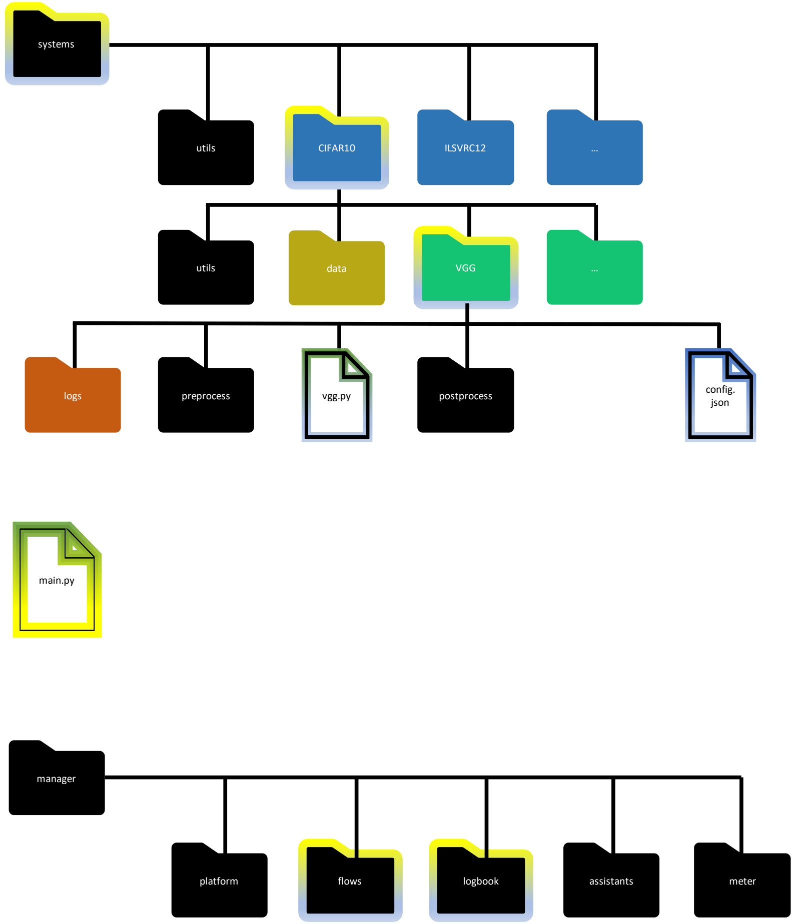


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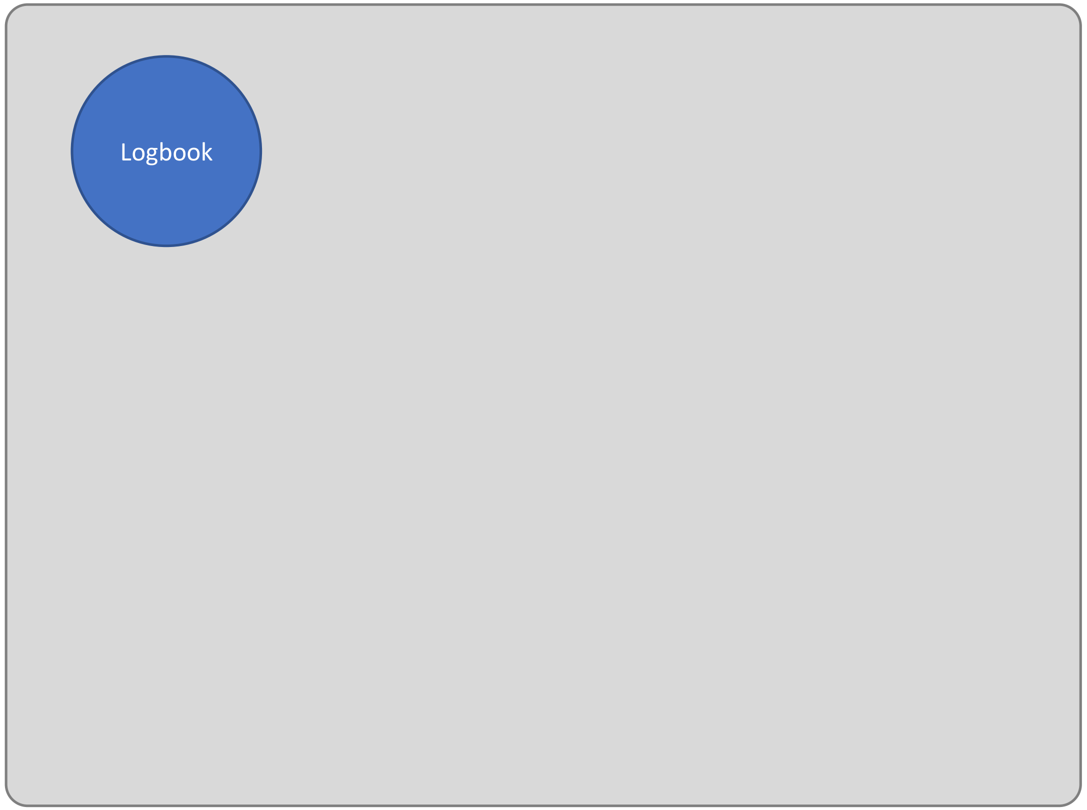

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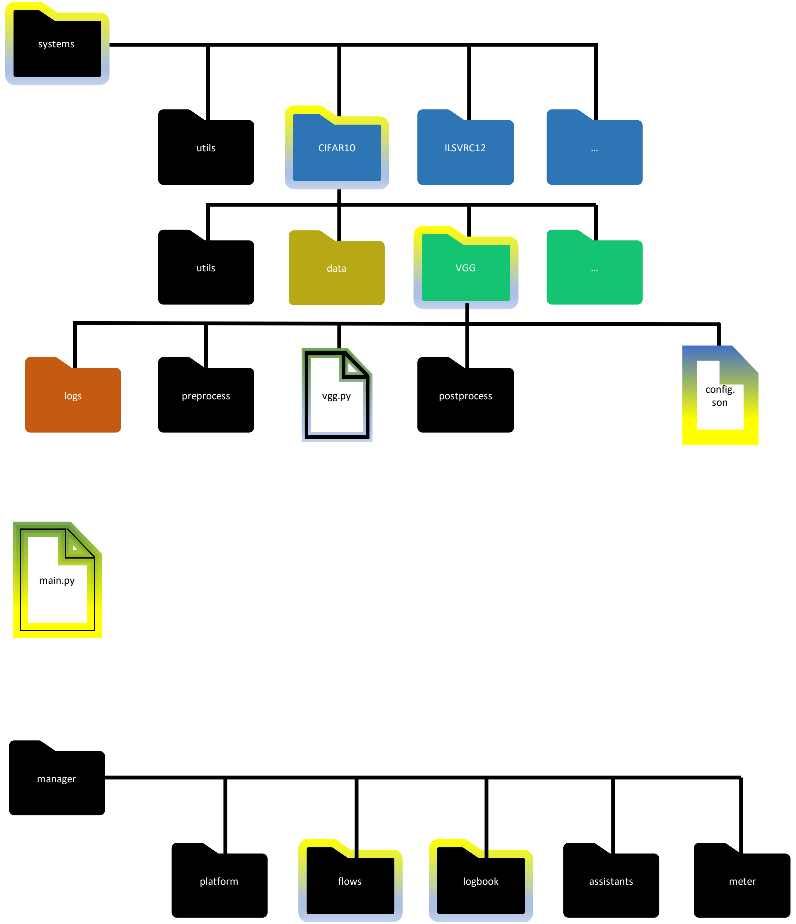


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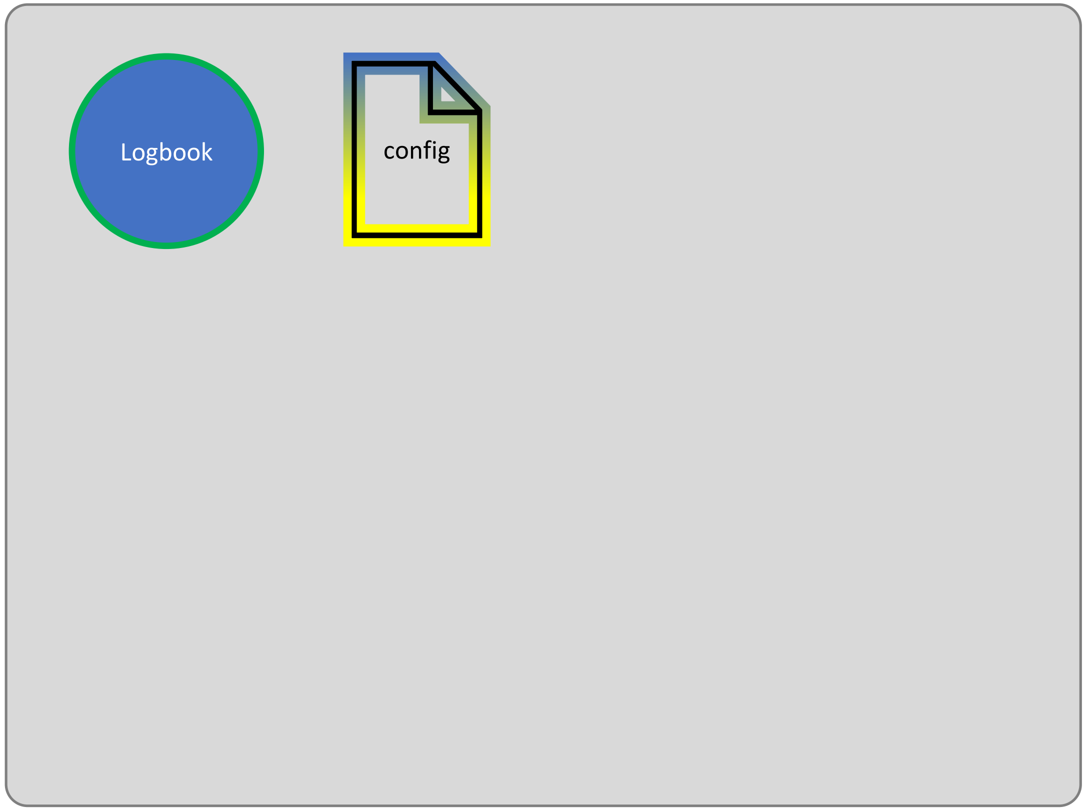

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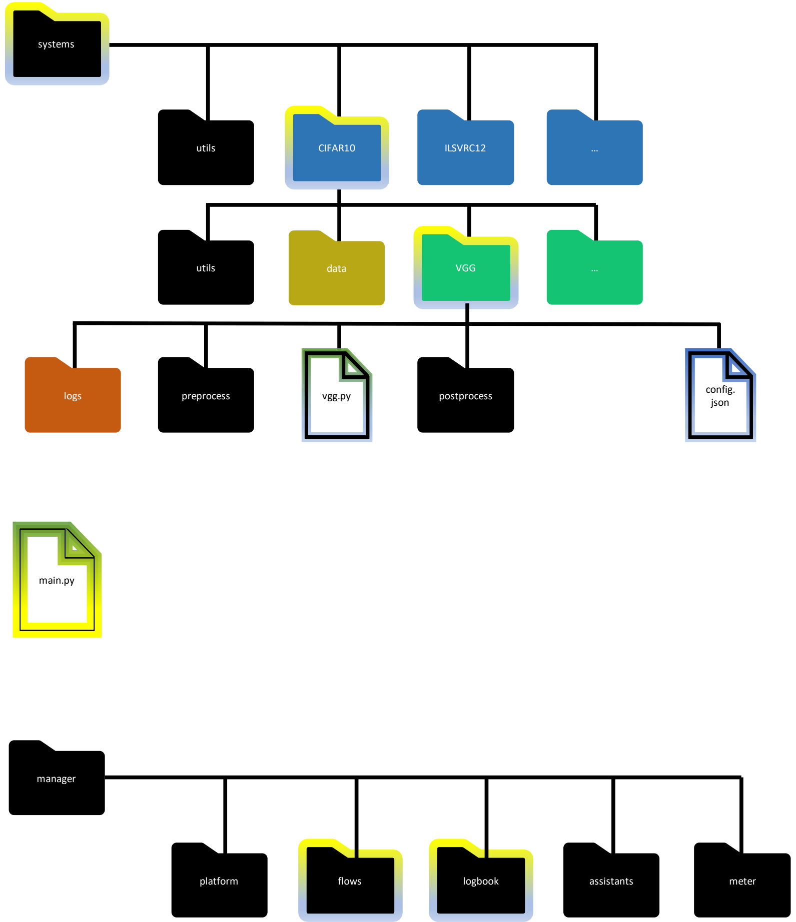


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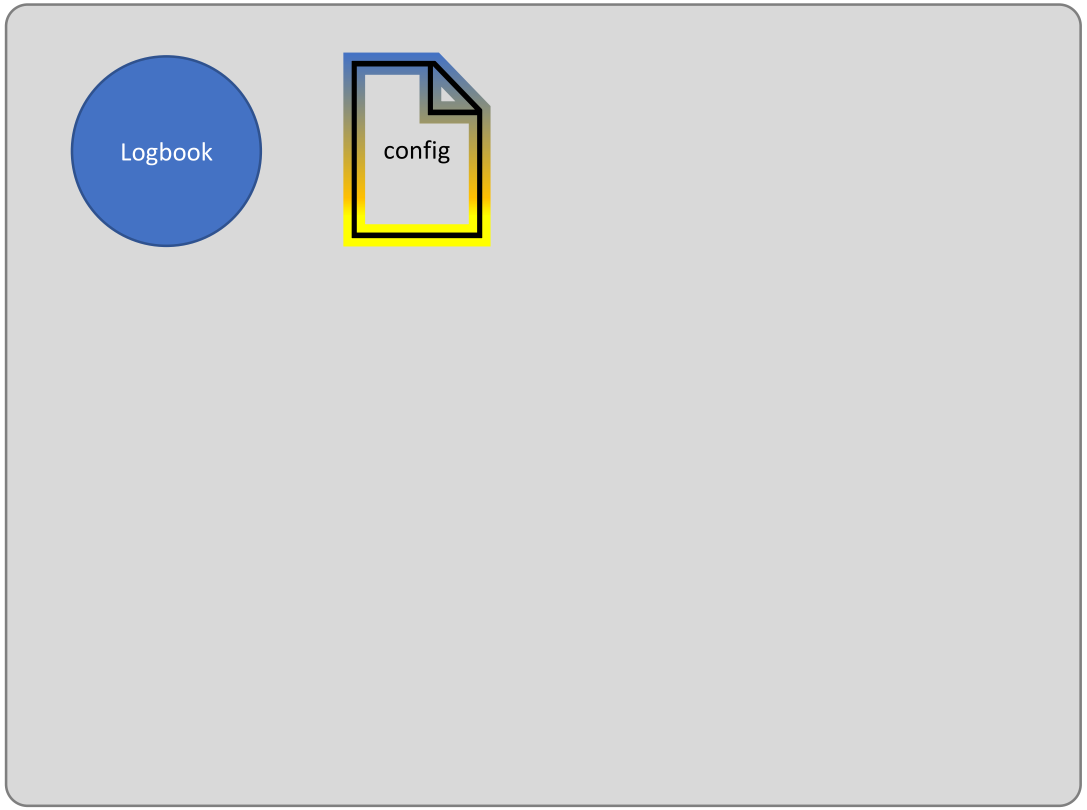

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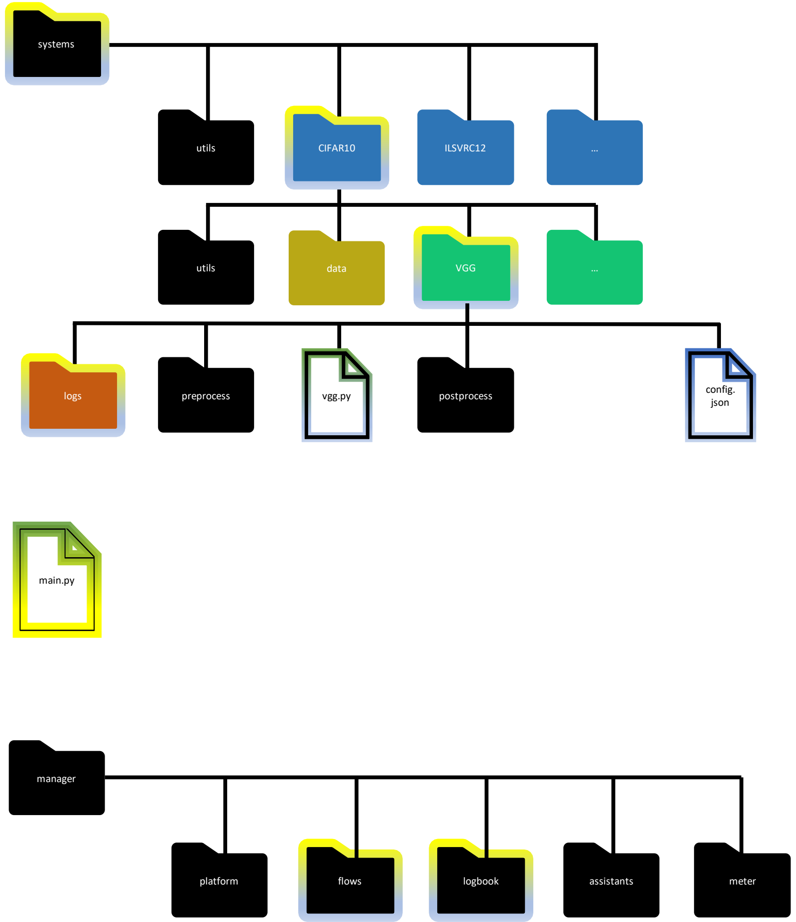


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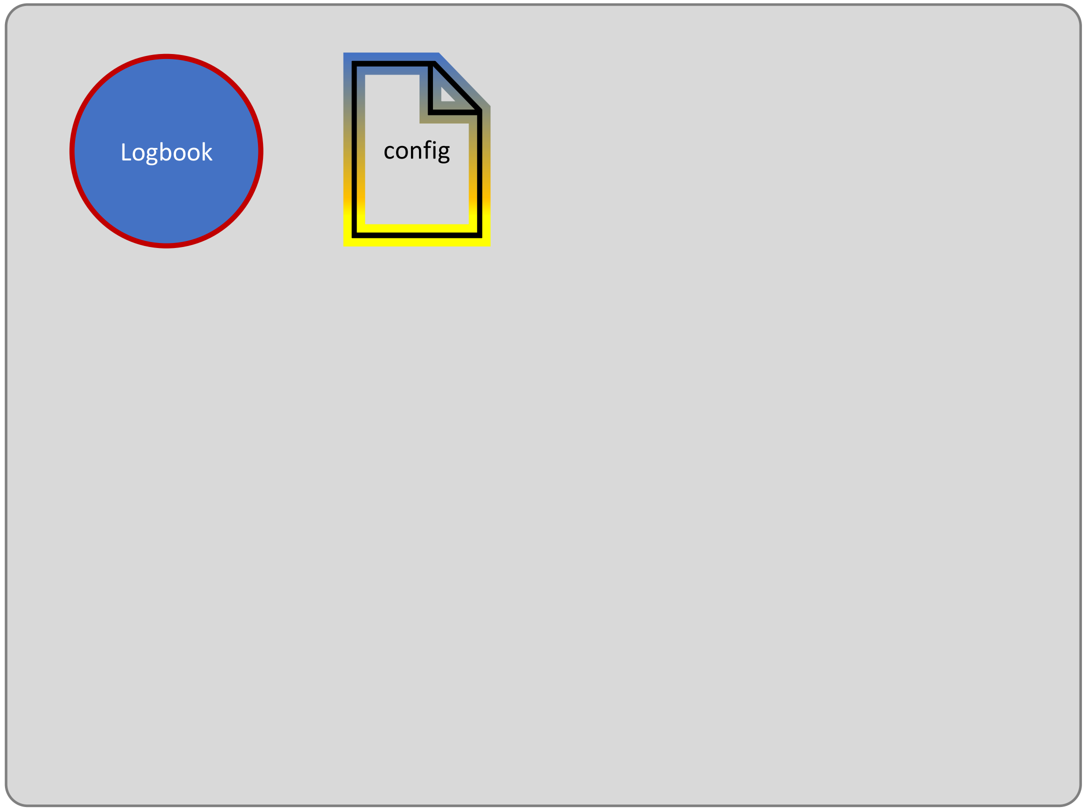

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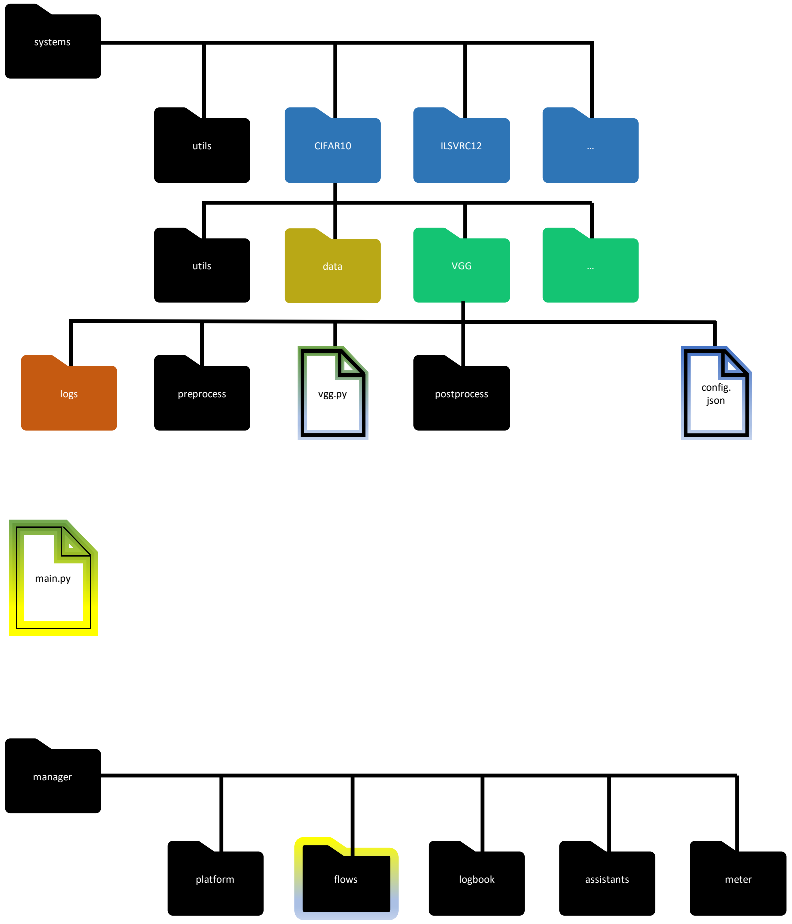


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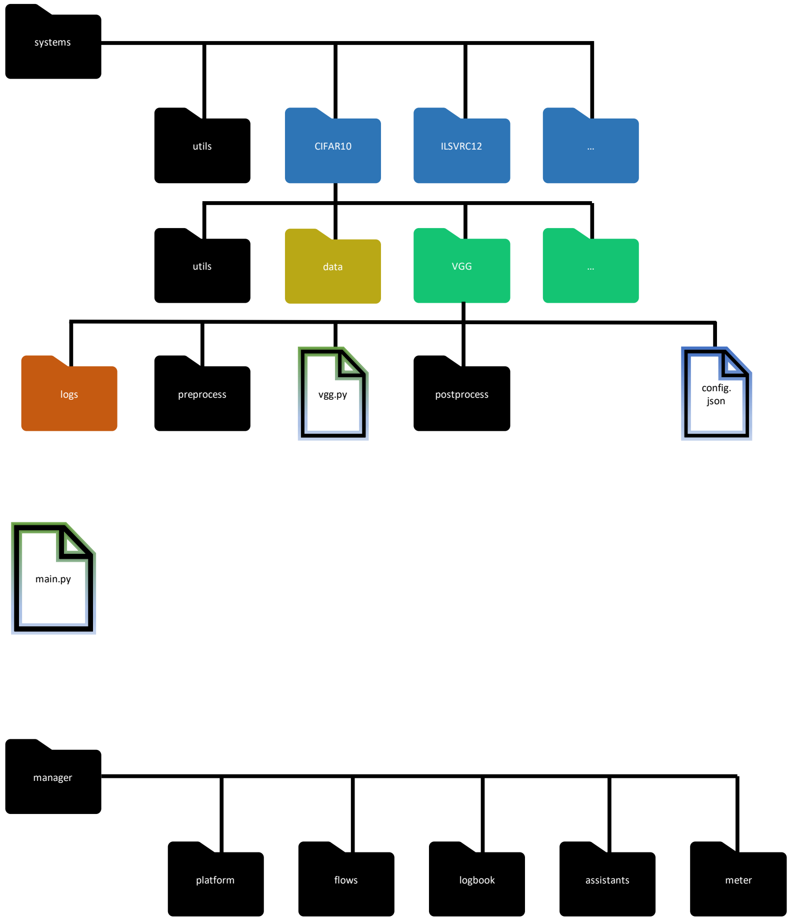


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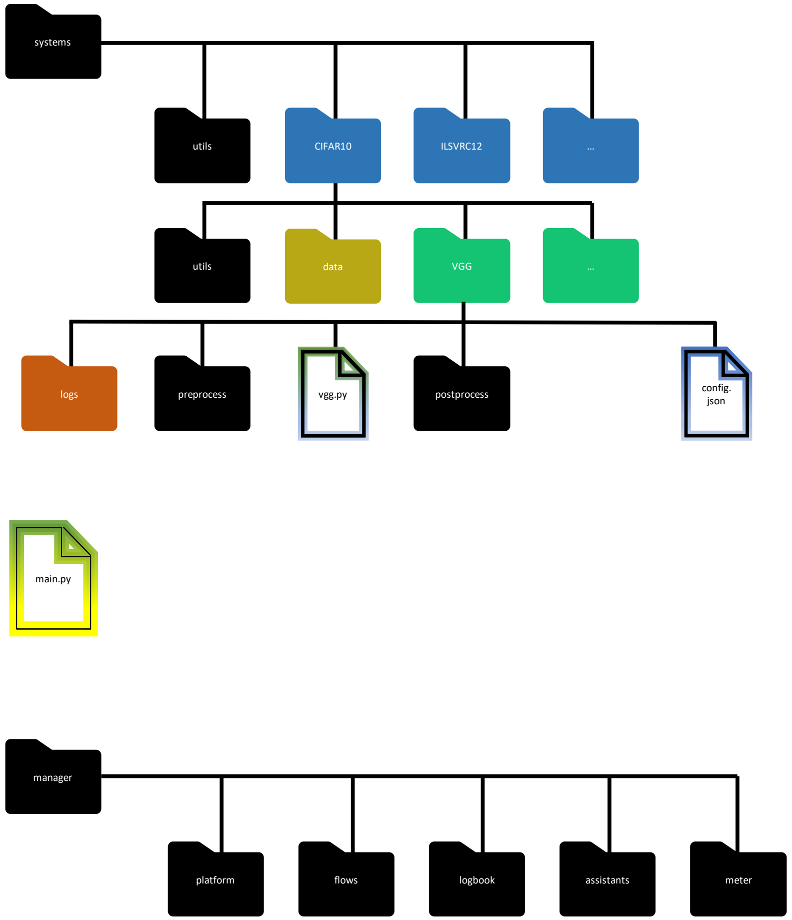


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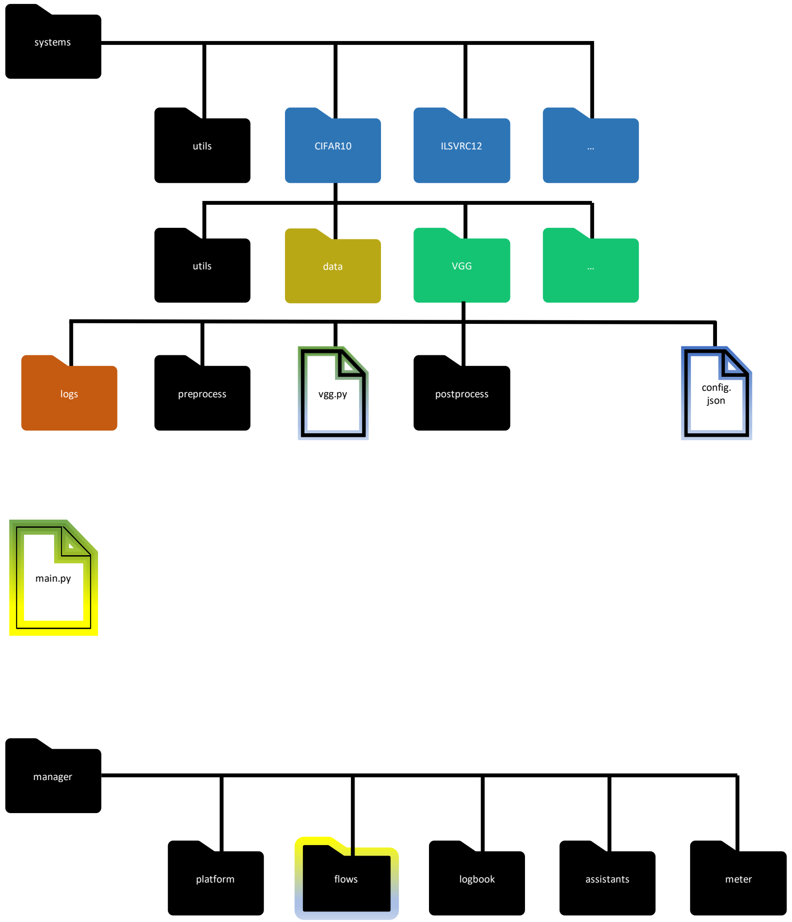


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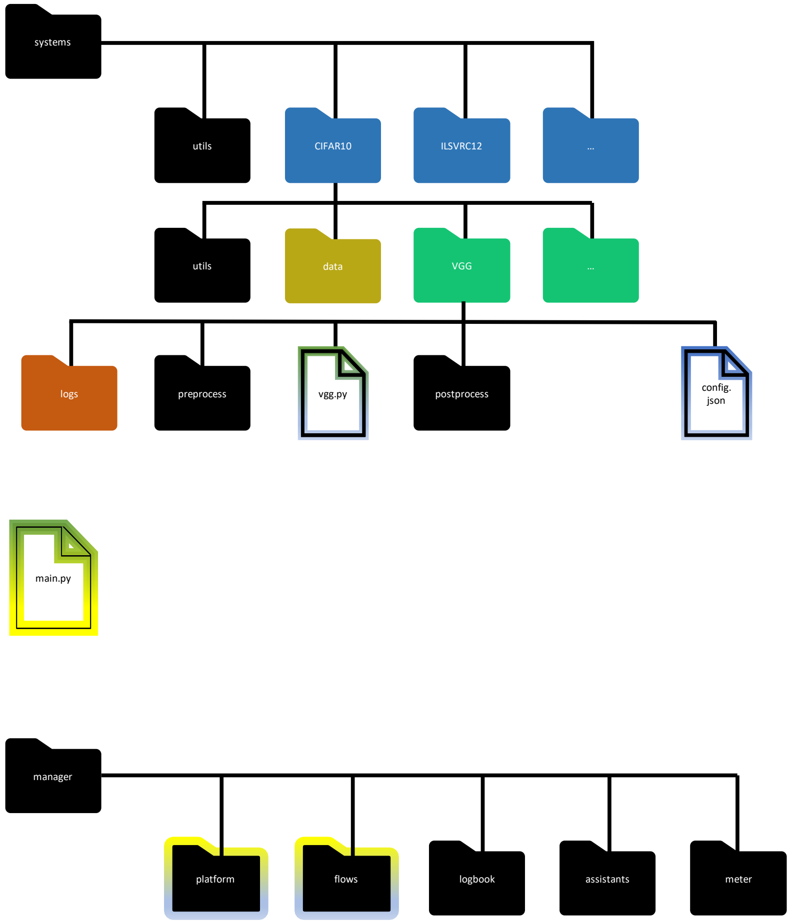


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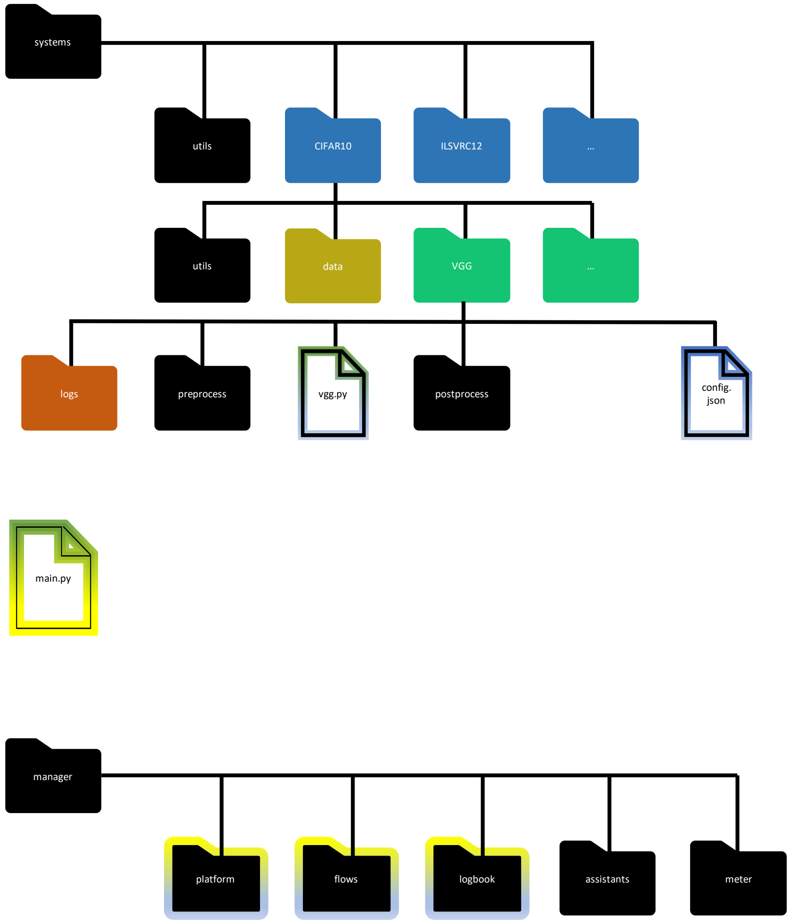


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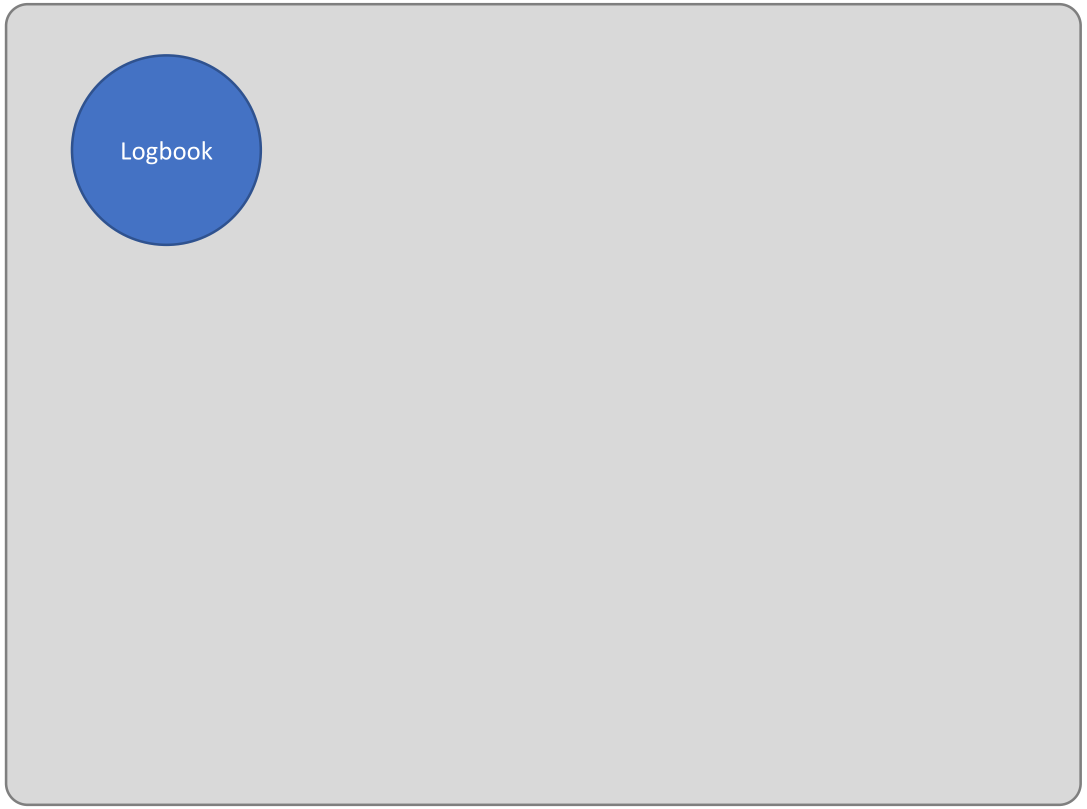

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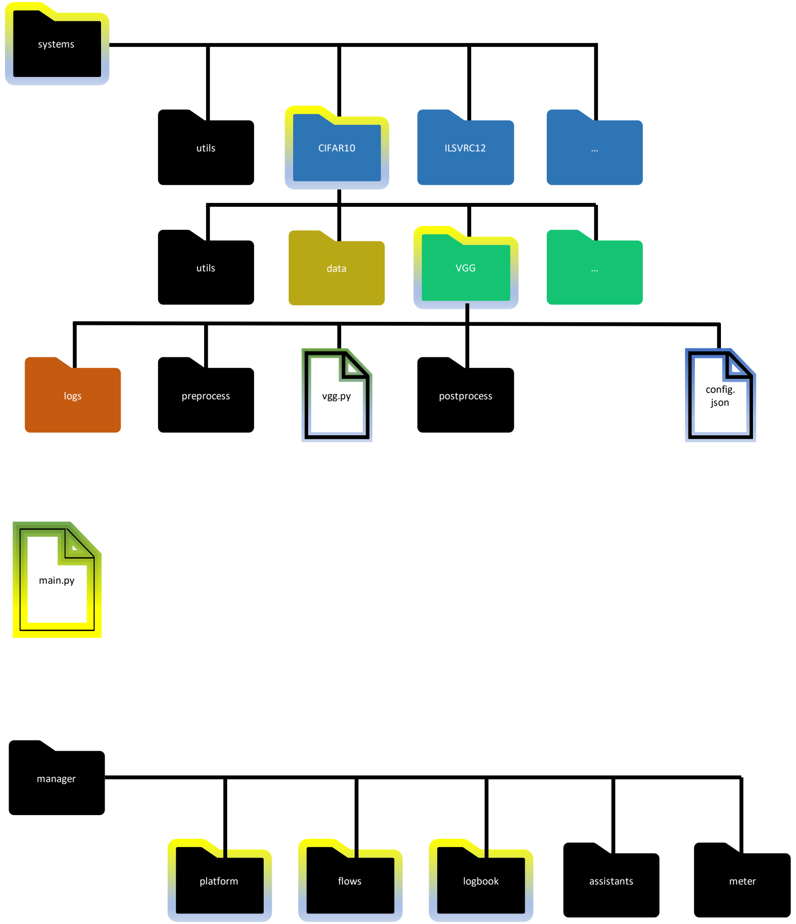


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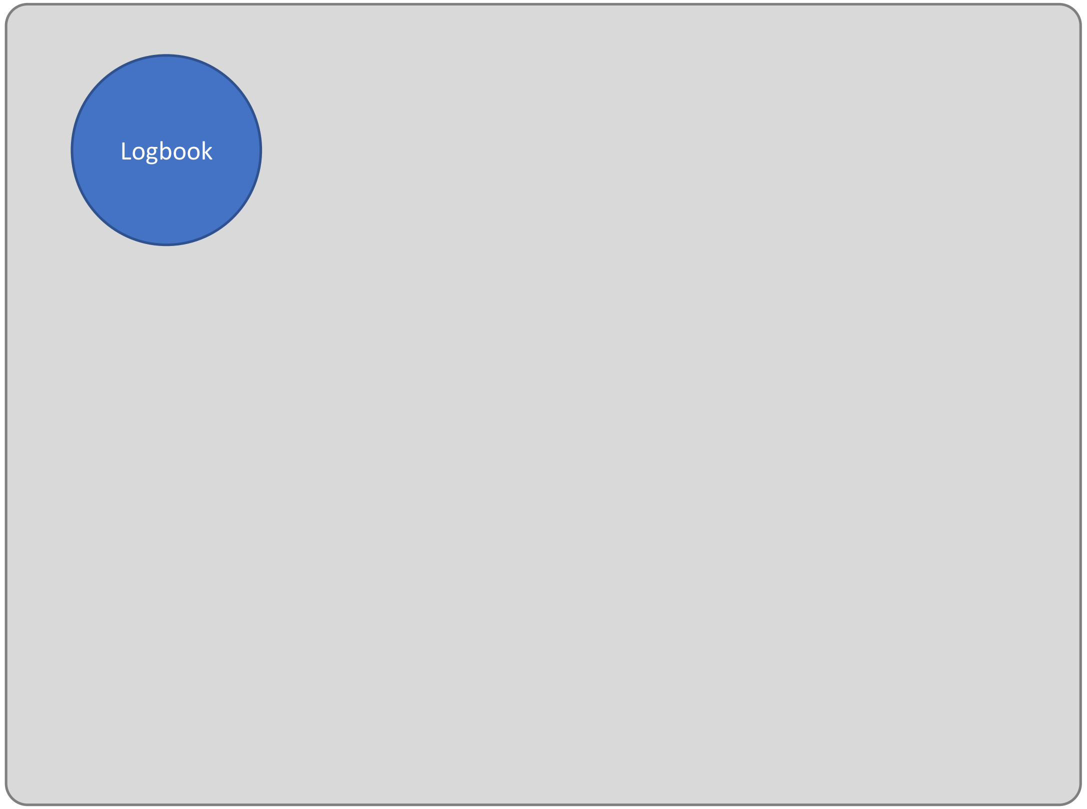

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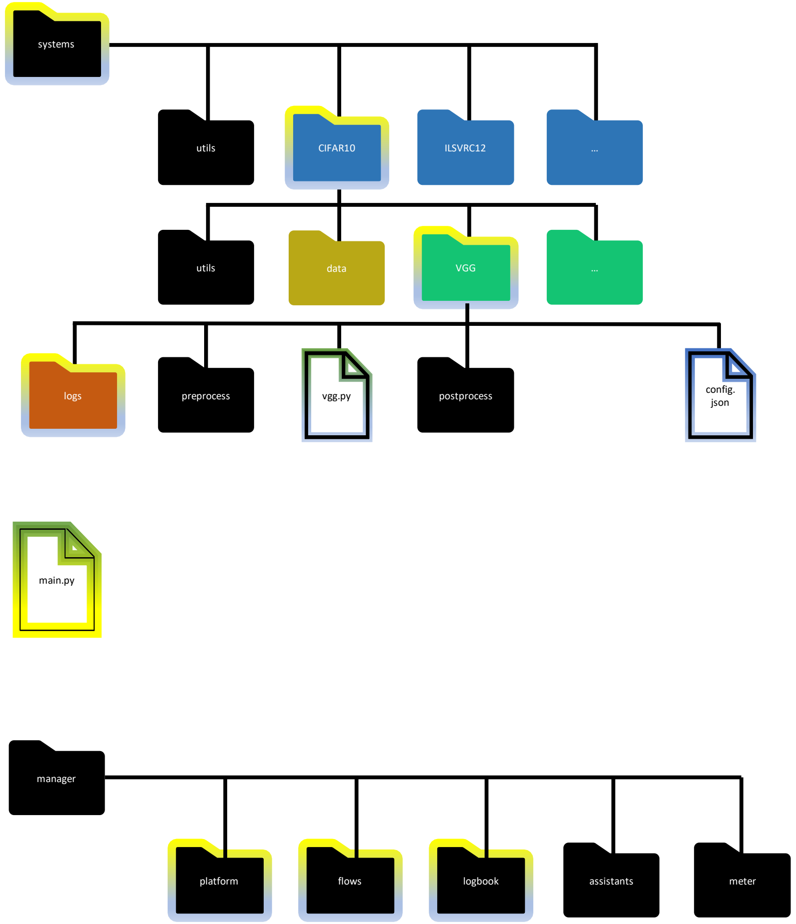


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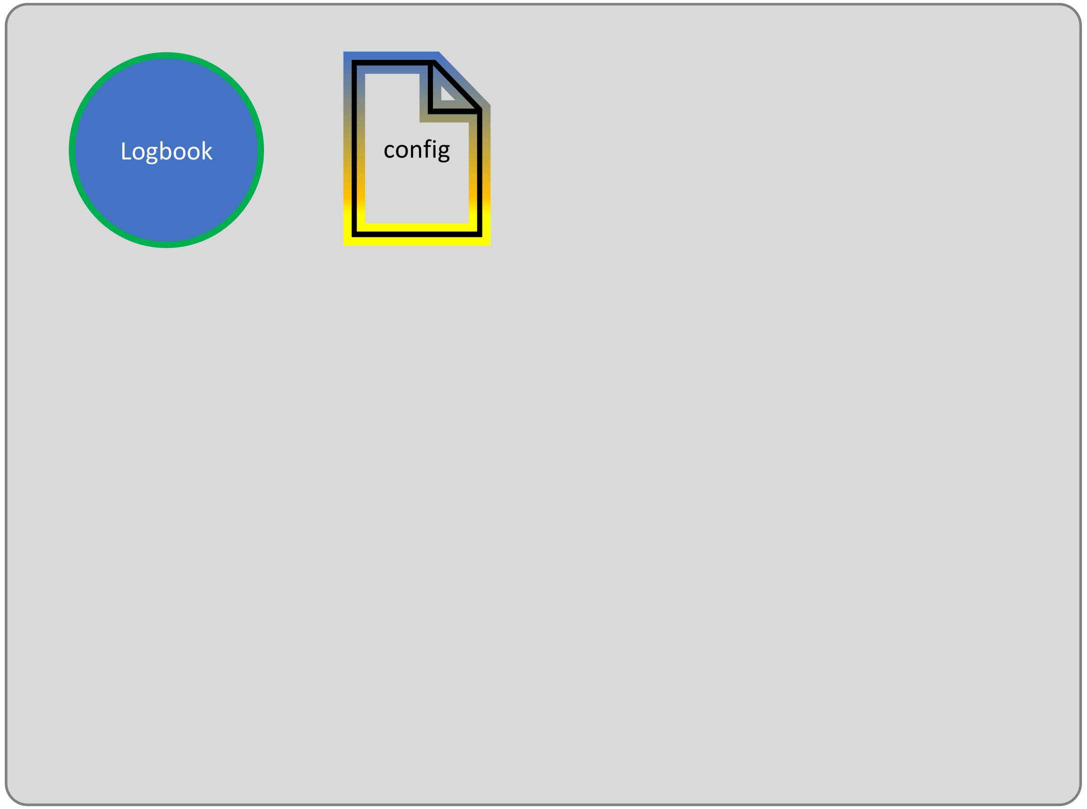

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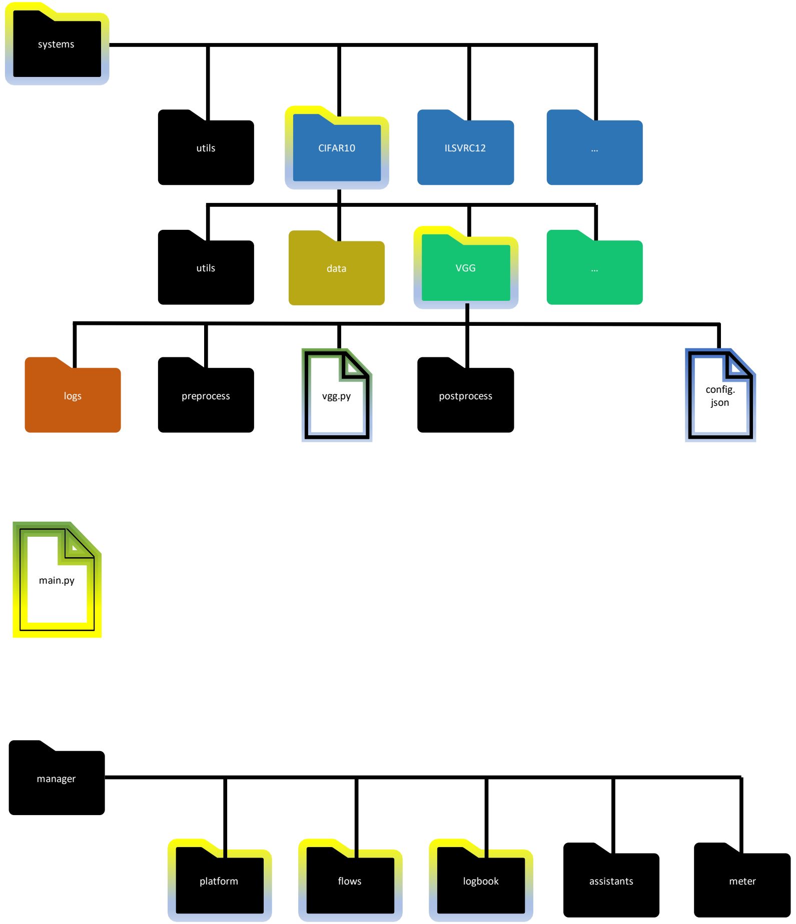


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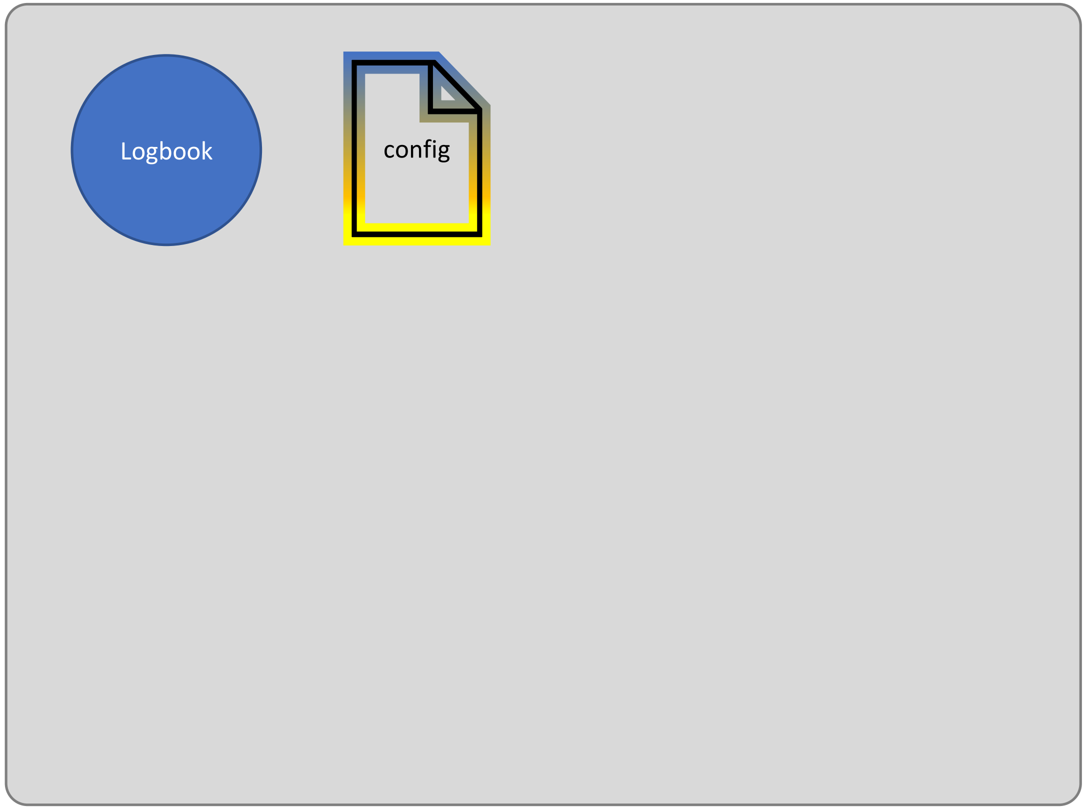

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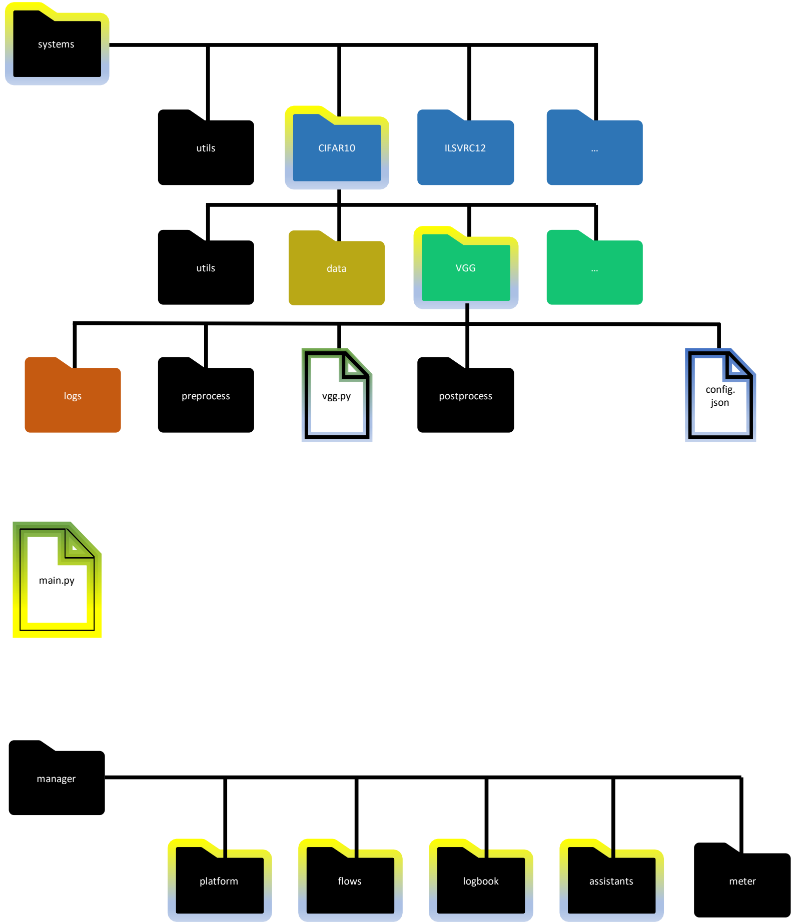


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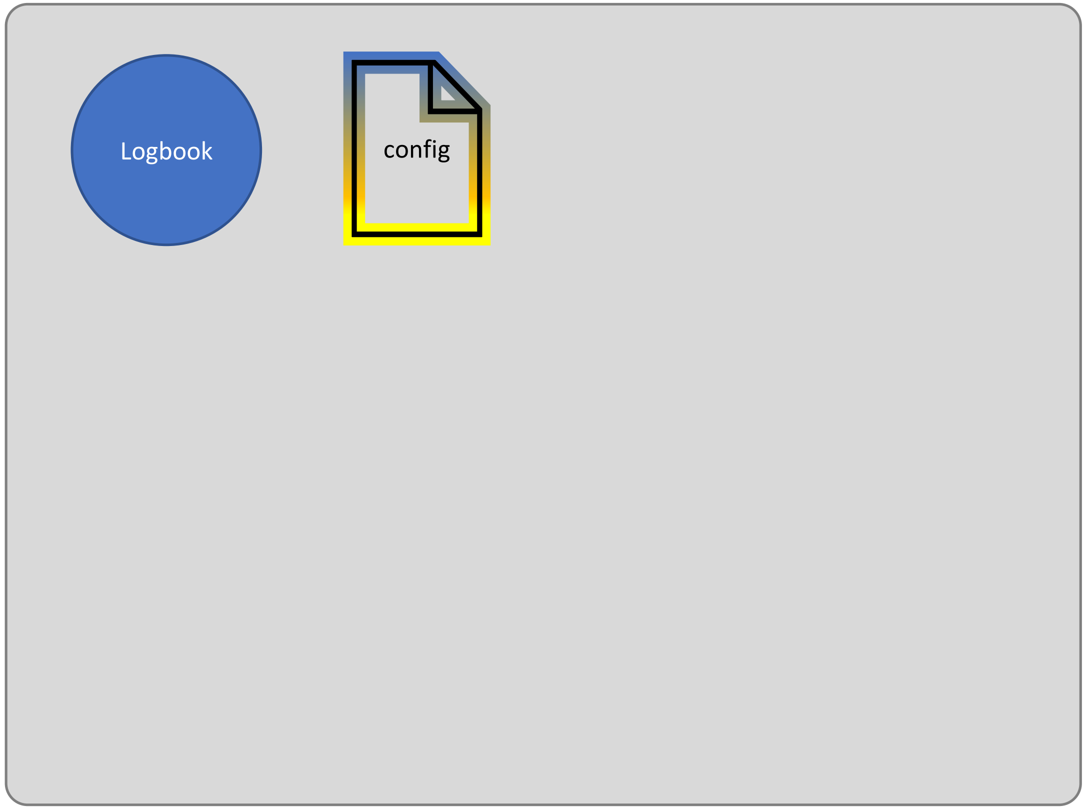

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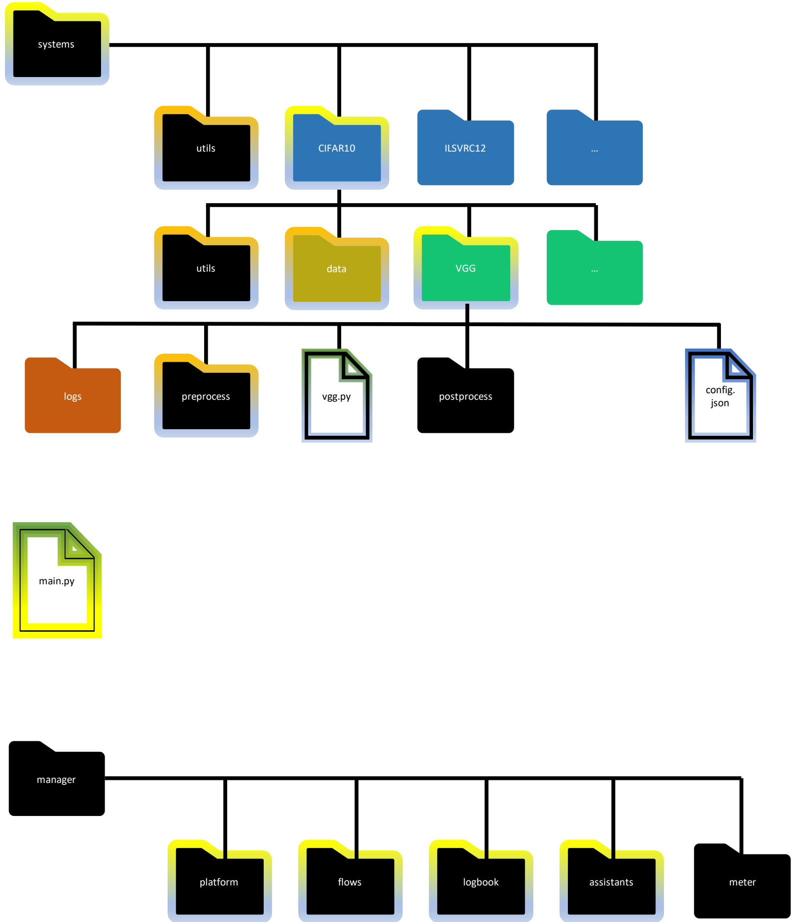


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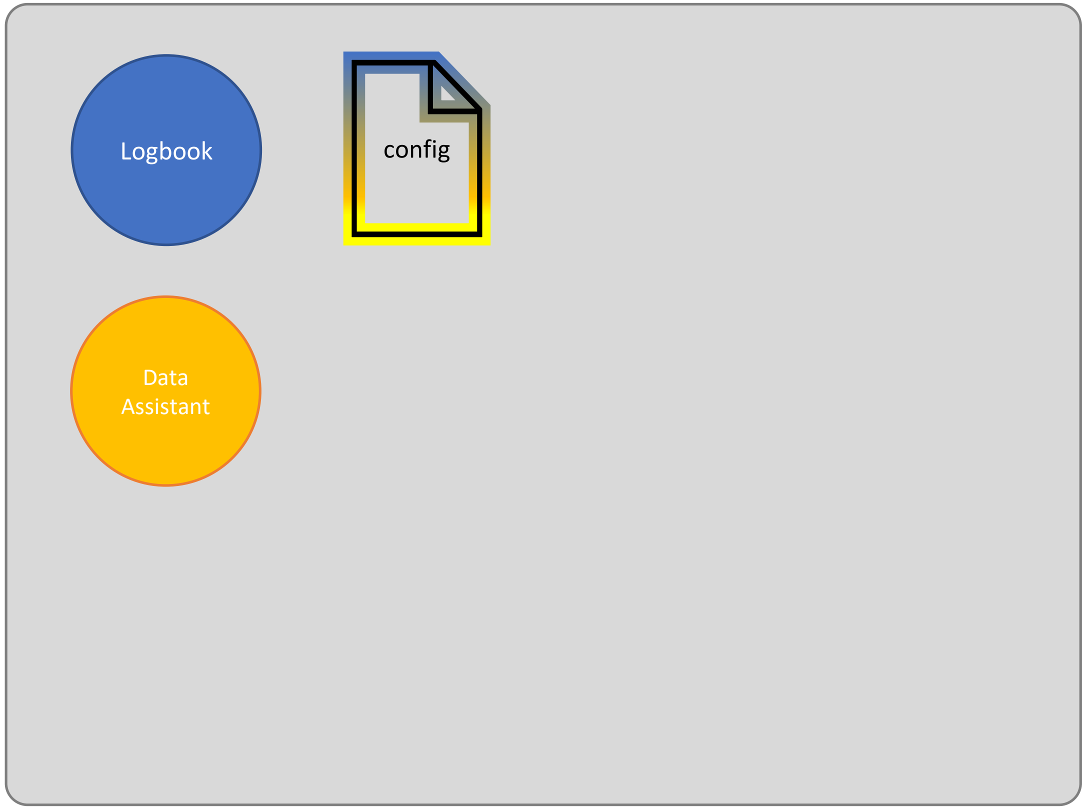

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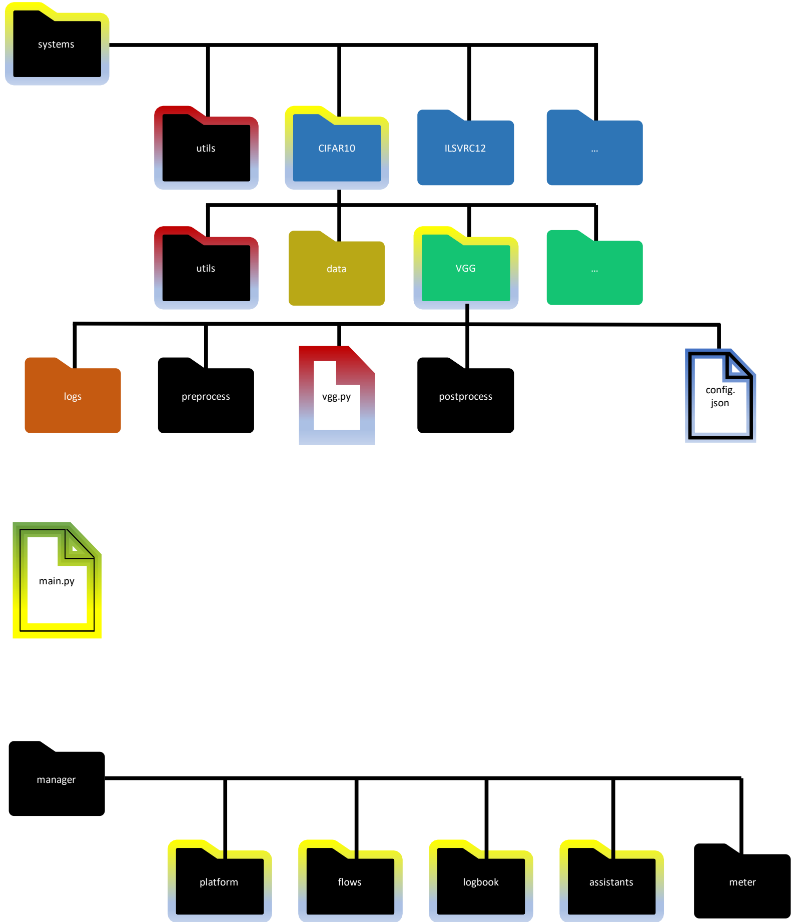


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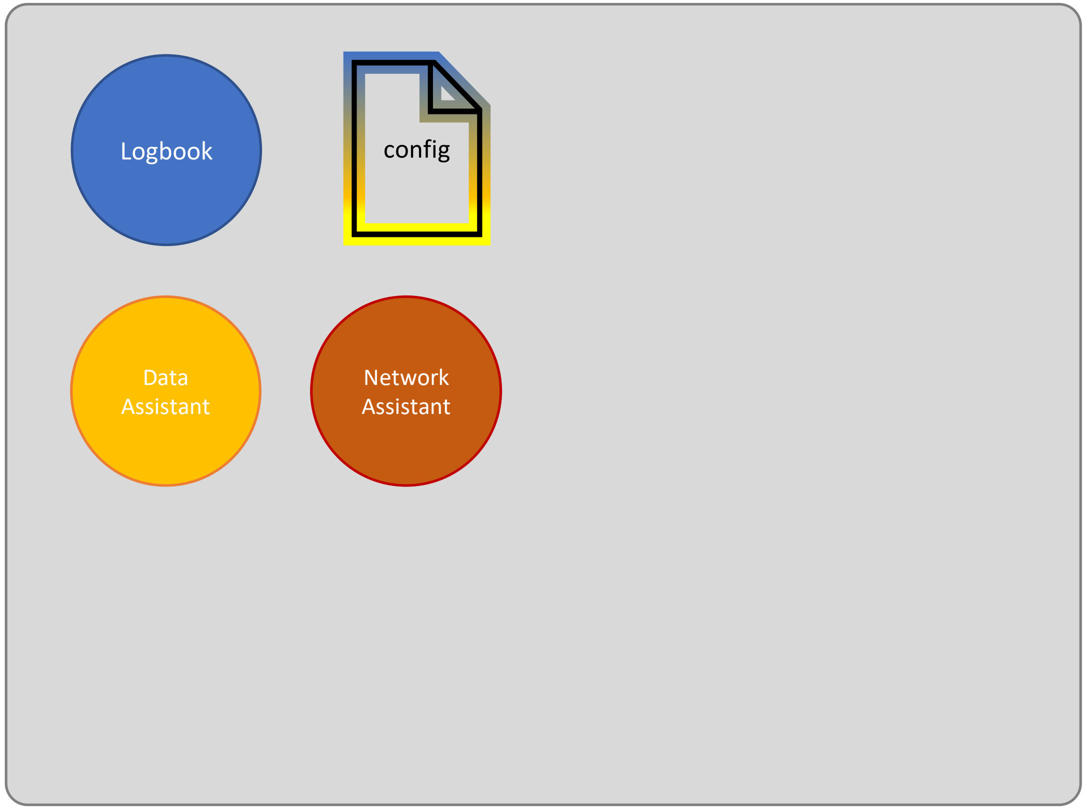

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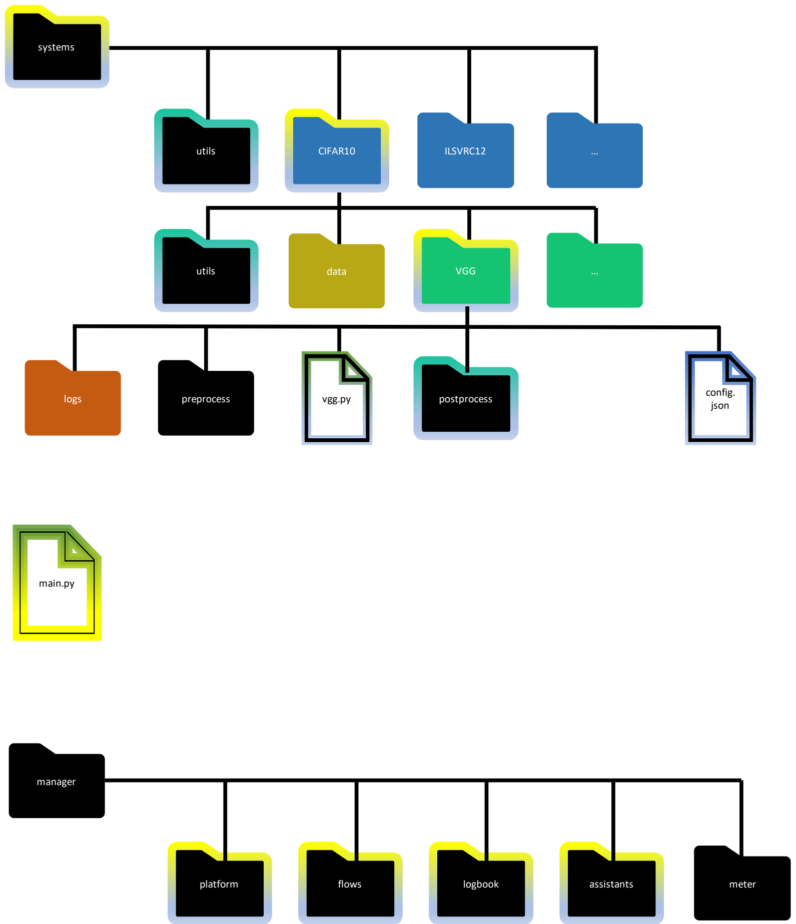


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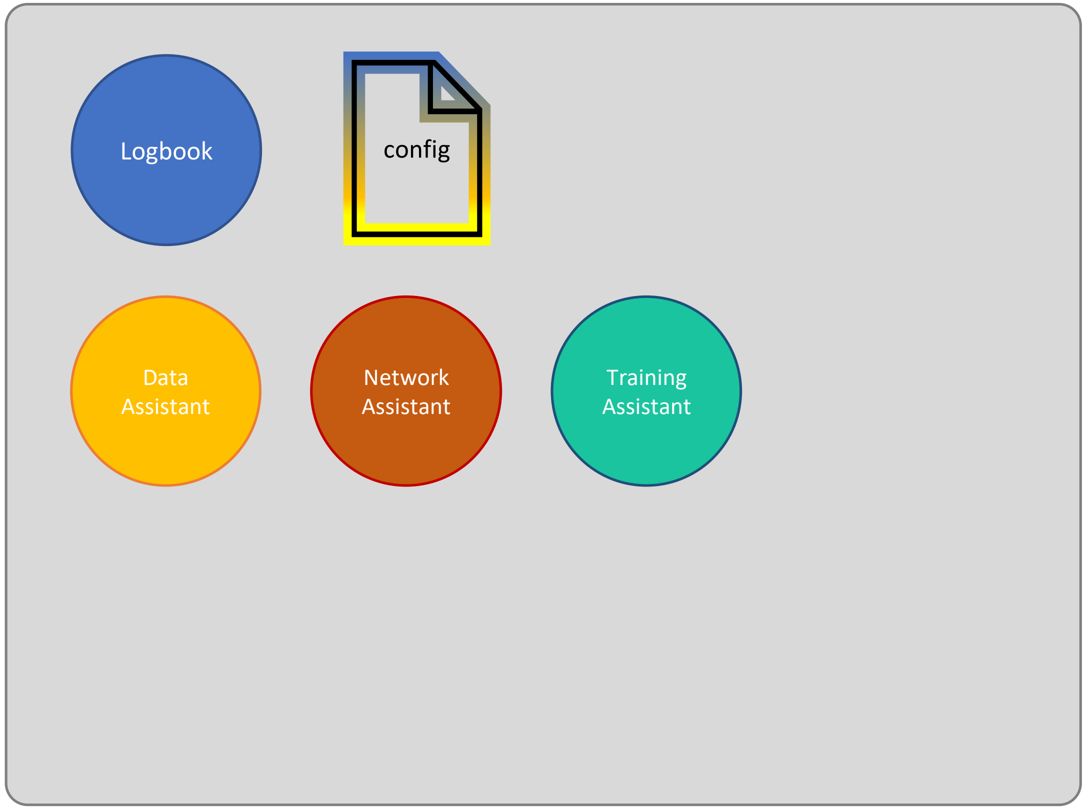

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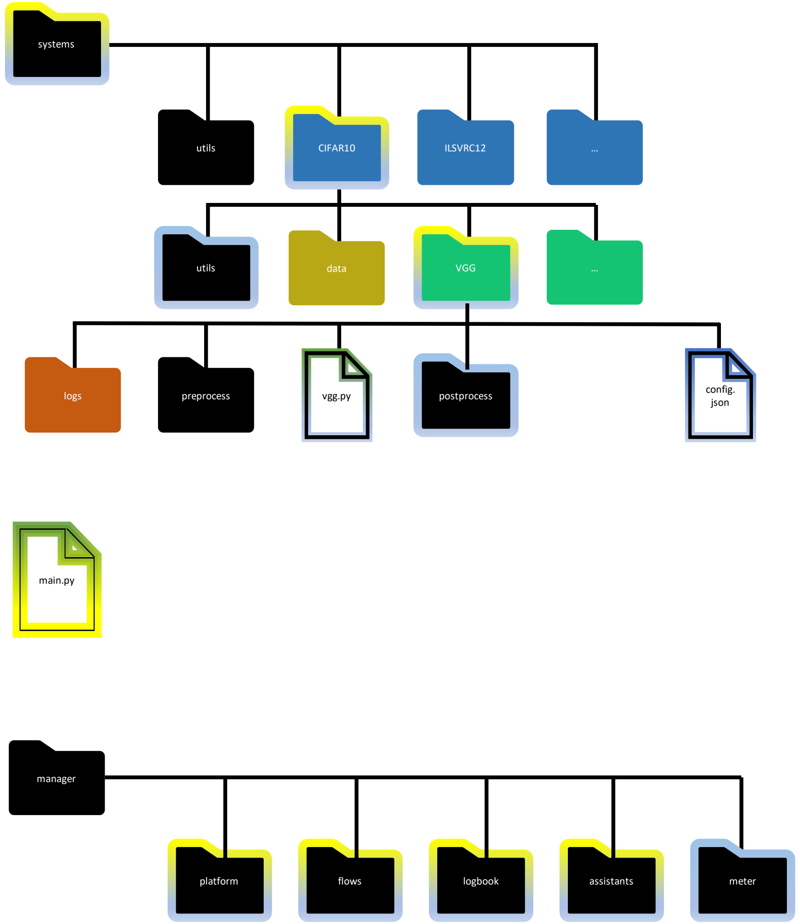


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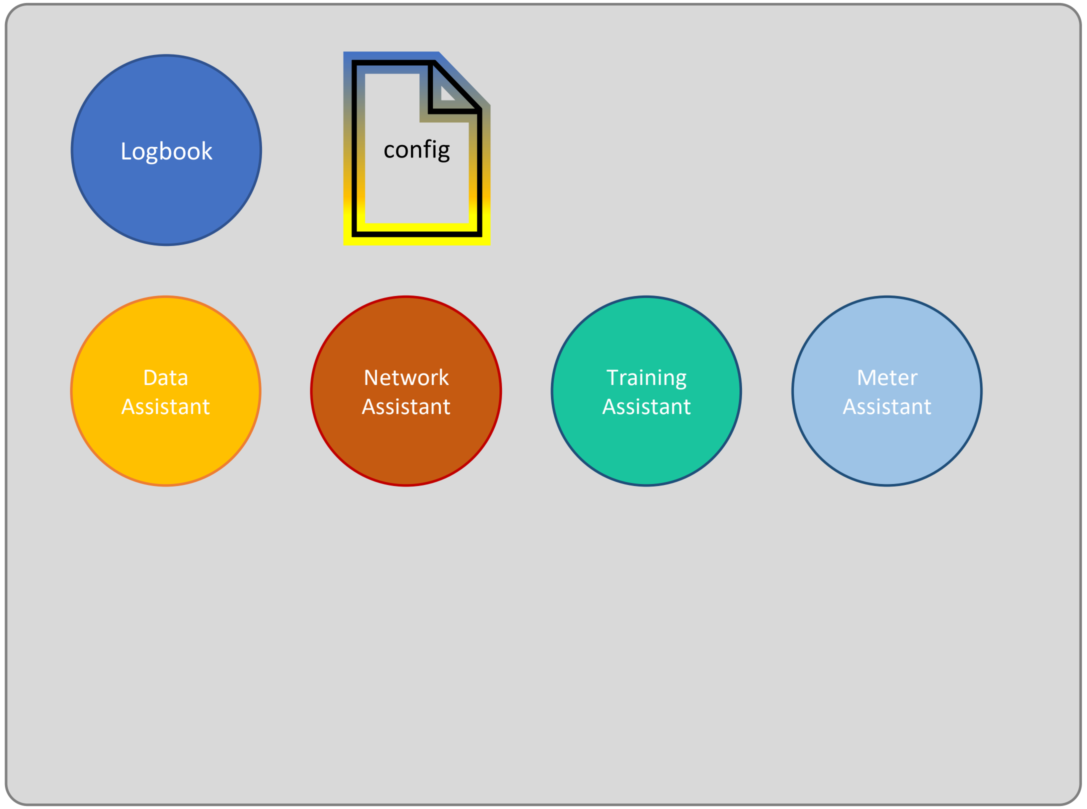

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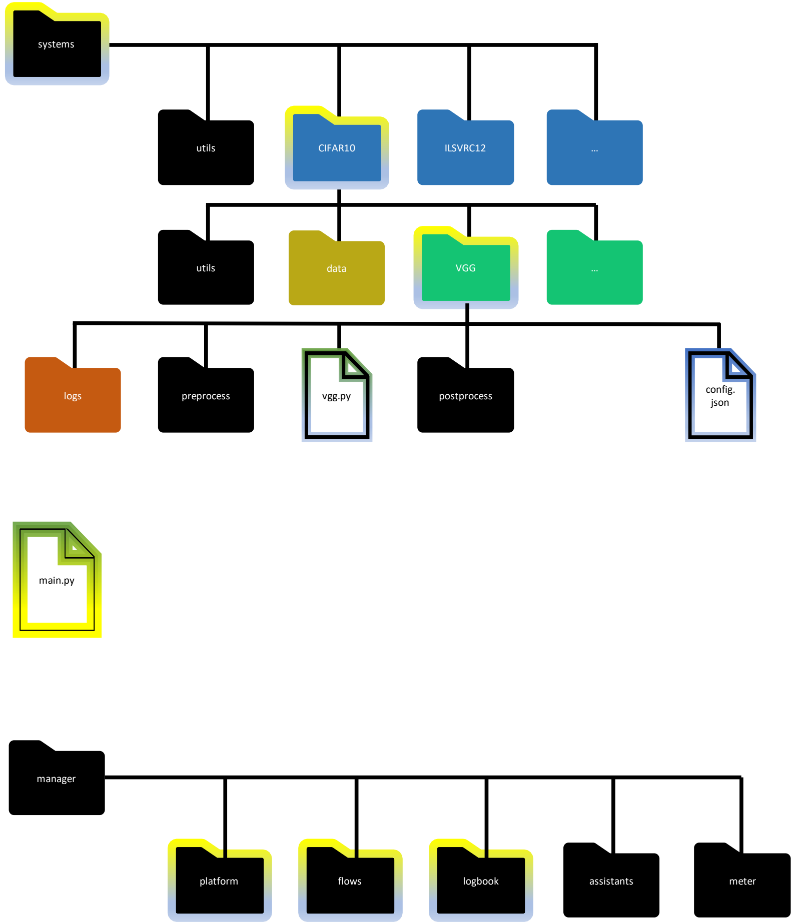


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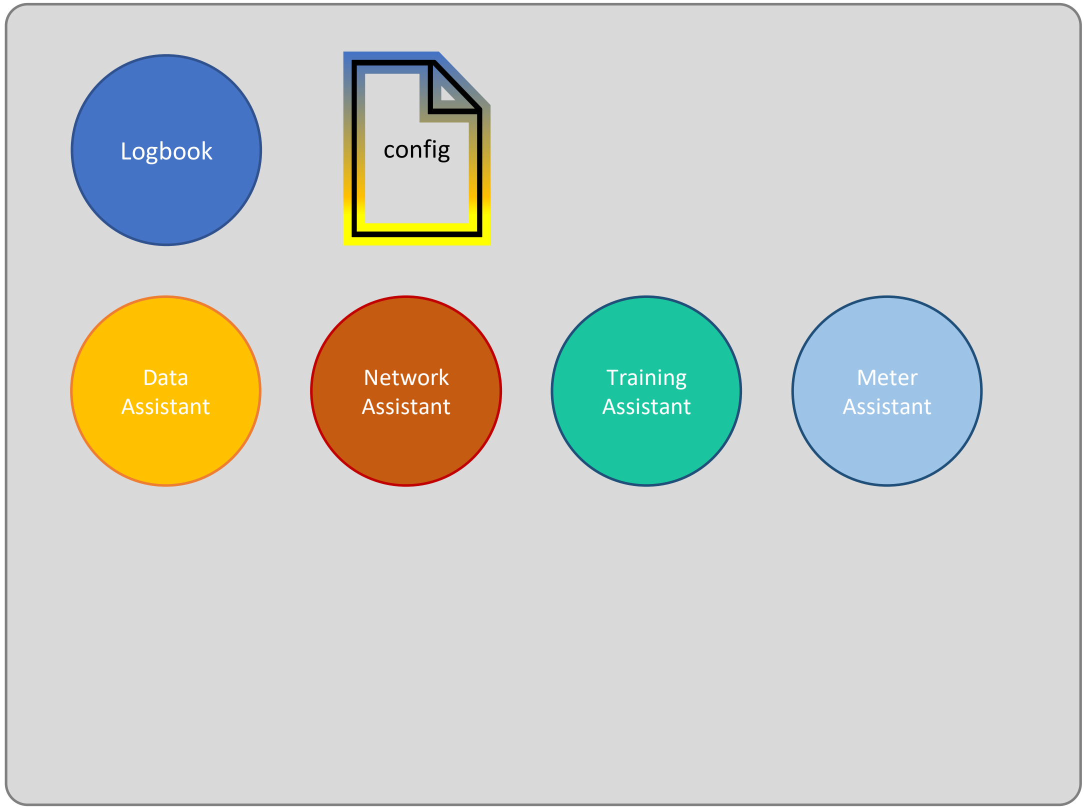

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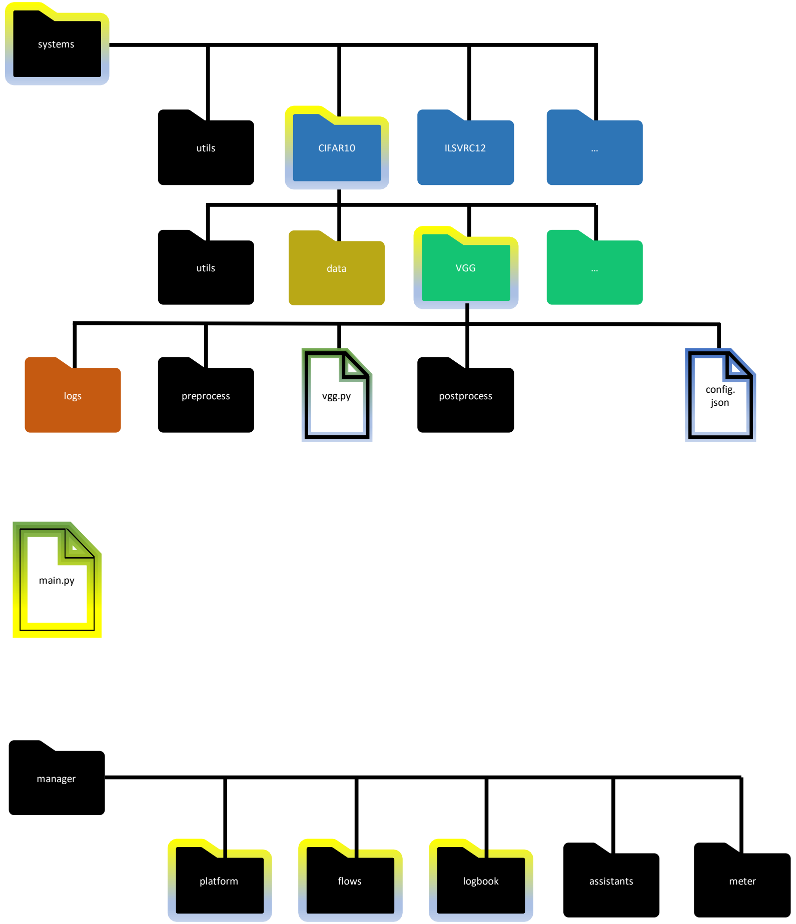


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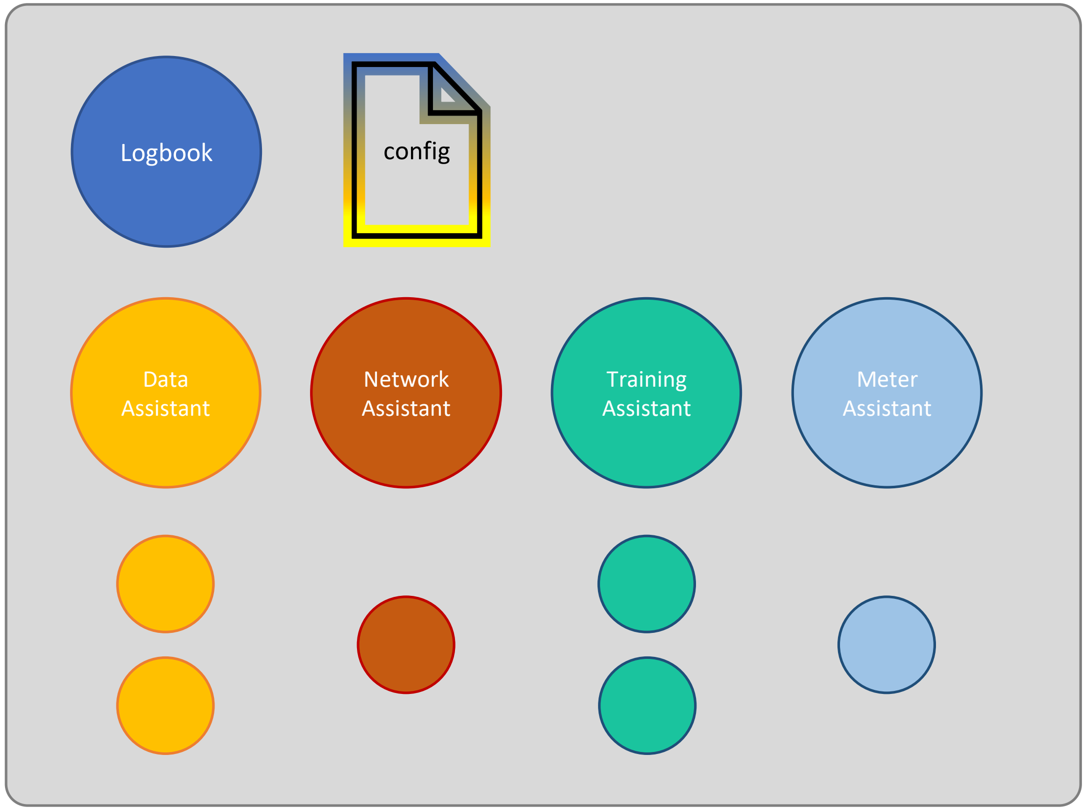

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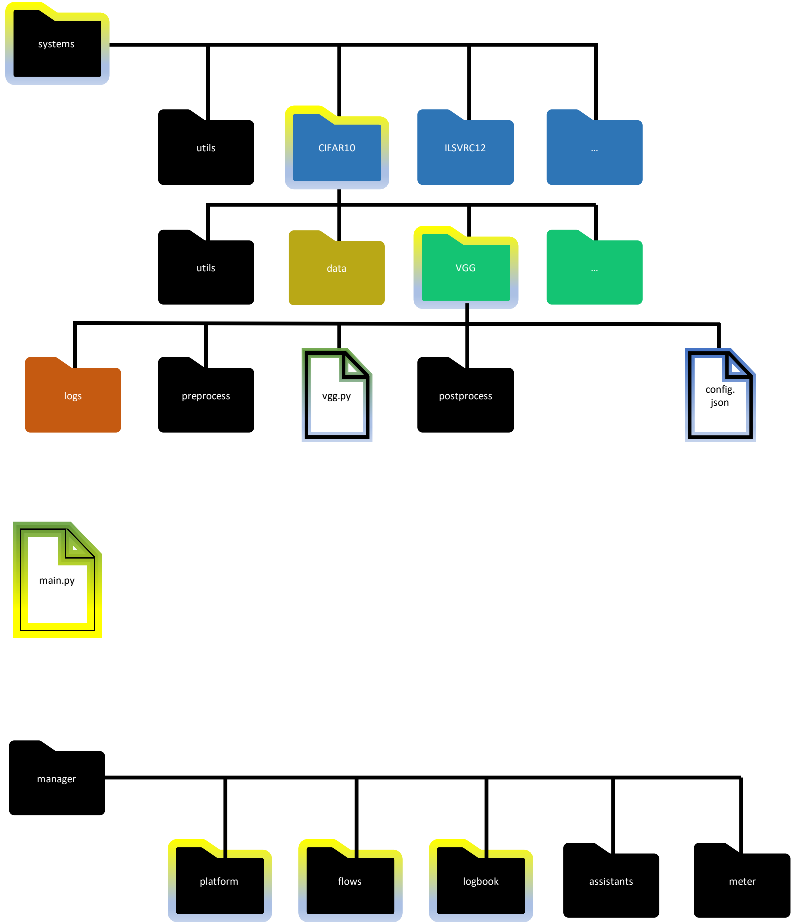


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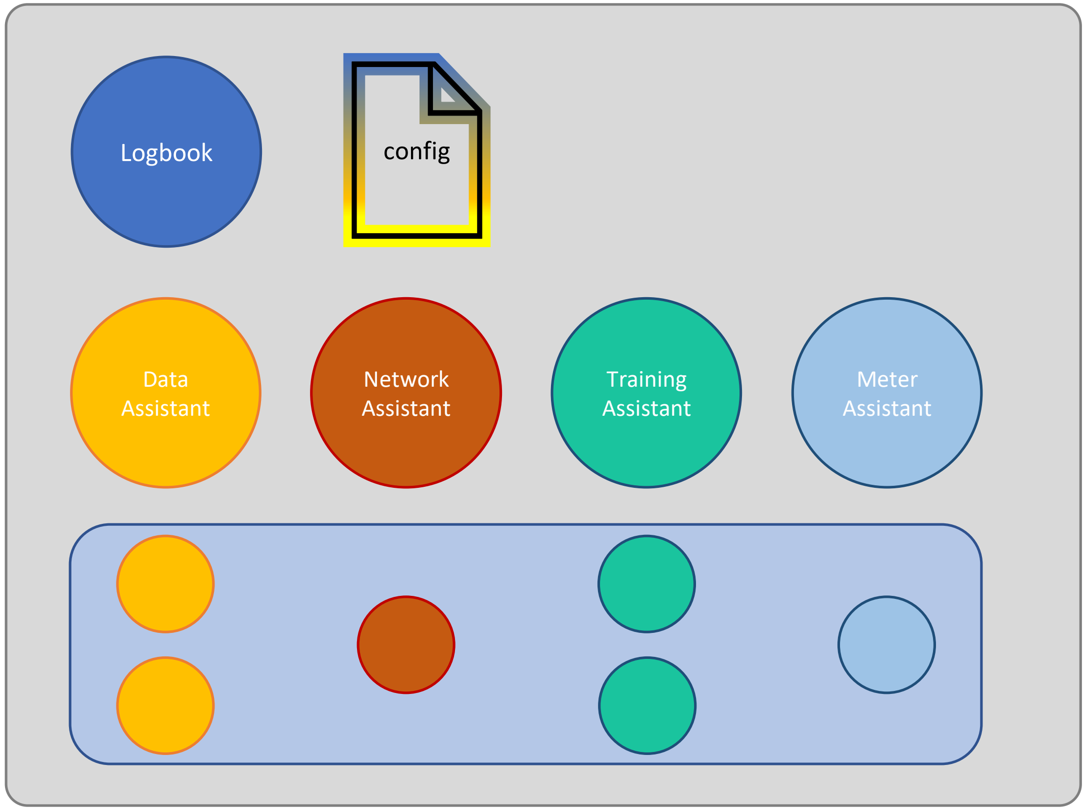

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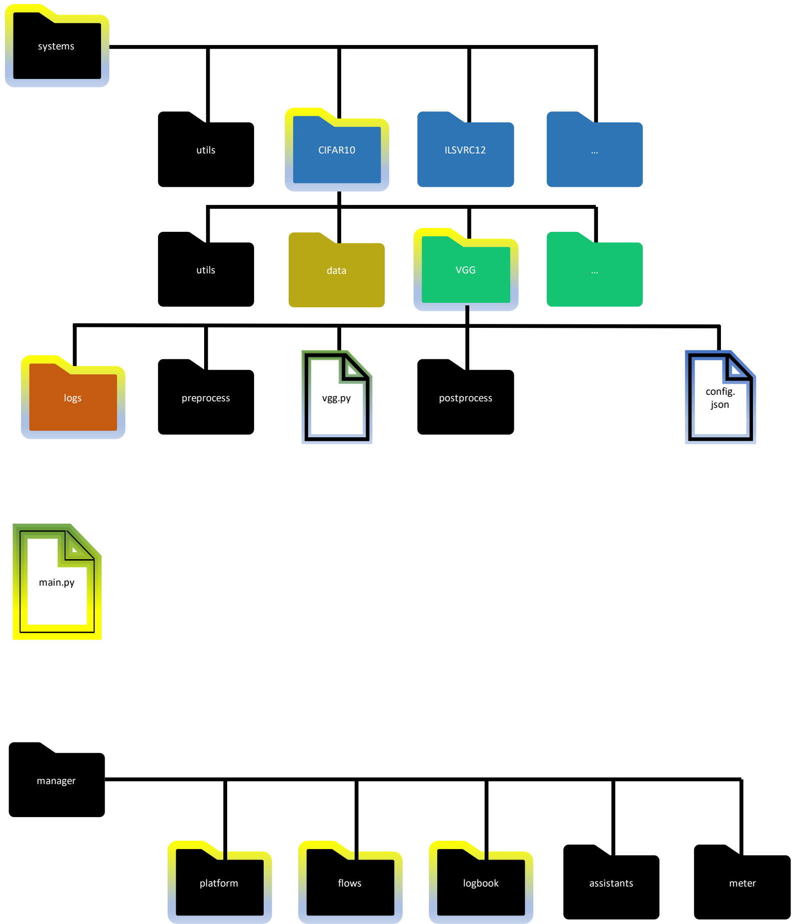


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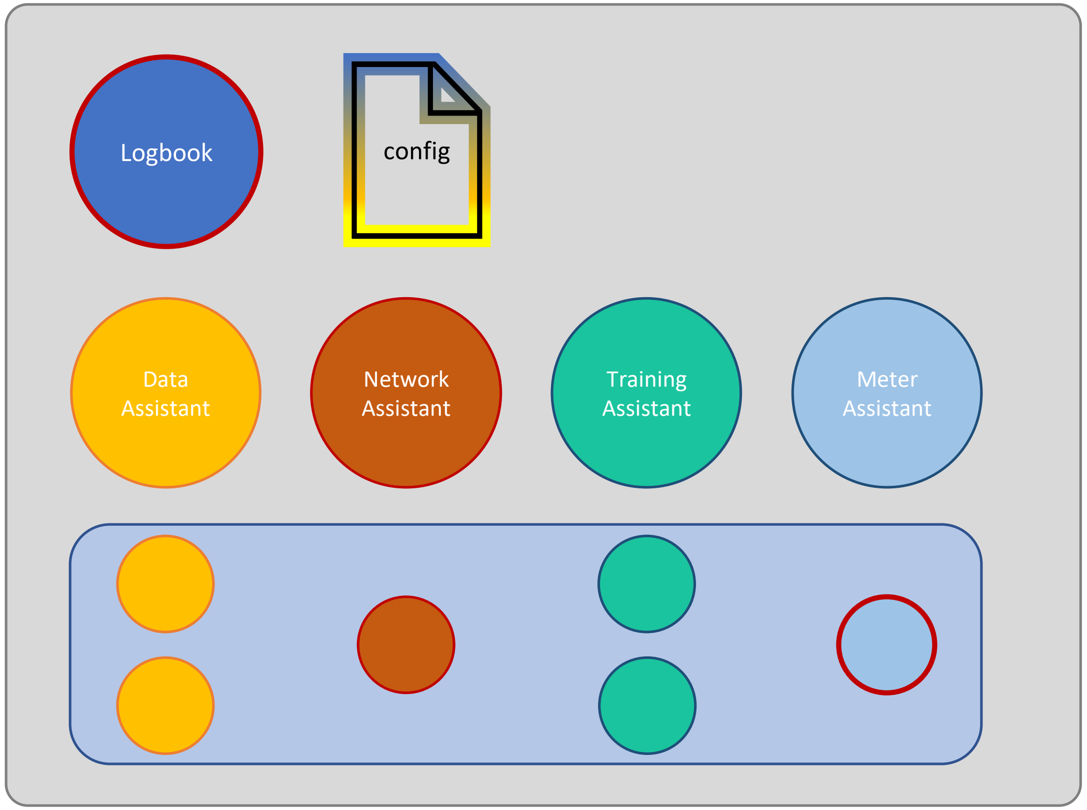

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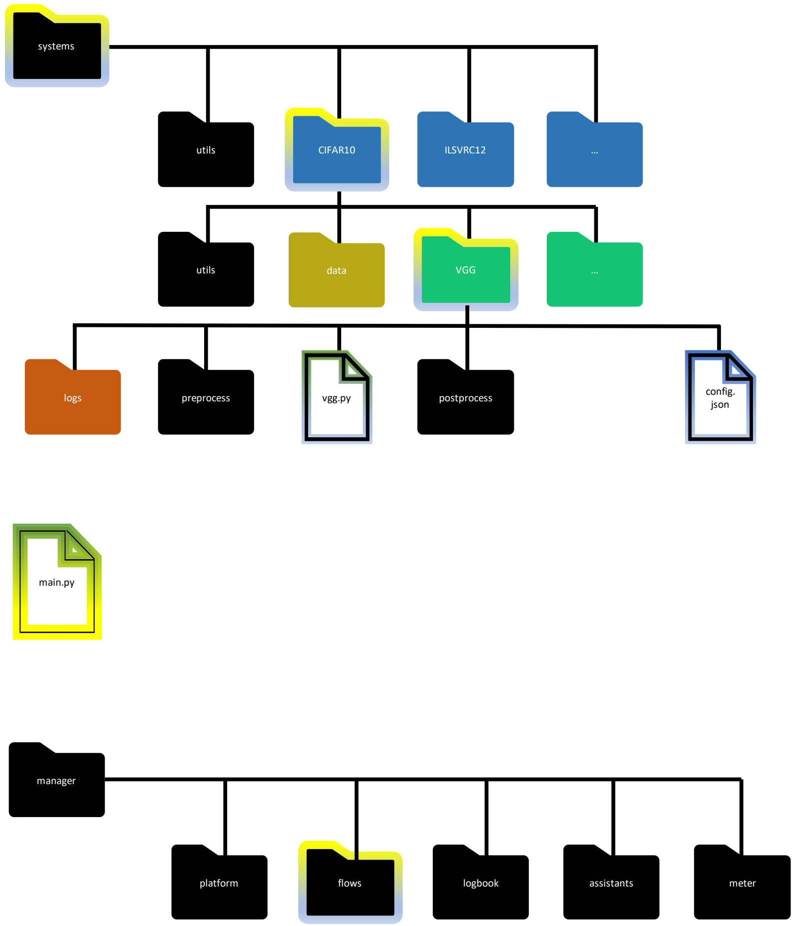


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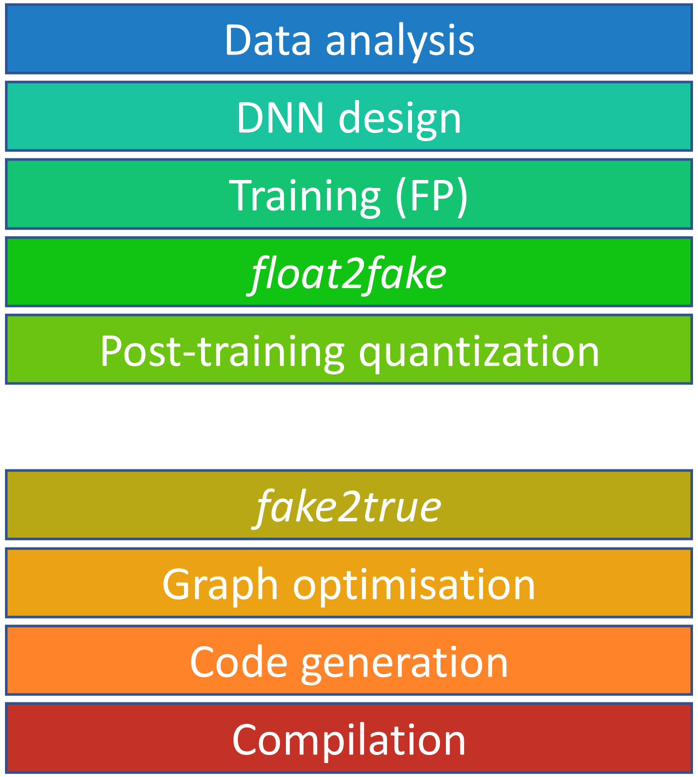
# QuantLab: usage overview

- Create a problem sub-package (remember to prepare the data!)
- Create a topology sub-package
- Write the working files:
  - Data pre-processing and loading
  - Network definition
  - Output post-processing

- Write the configuration file that describes how to instantiate the system
- Run the `configure` flow
- Run the `training` flow

**ITERATE UNTIL YOU ARE SATISFIED!**

# QNNs: a HW/SW co-design problem




**Platform-agnostic**

- **Data analysis**: how can we model the data problem?
- **DNN design**: which network topology can work best?
- **Training**: backpropagation + SGD

## Platform-aware

- ***float2fake*** conversion
- **Post-training quantization** algorithm (w/o fine-tuning)
- ***fake2true*** conversion

**Platform-specific**

- **Graph optimisation**: ONNX graph (e.g., tiling, “node fusion”)
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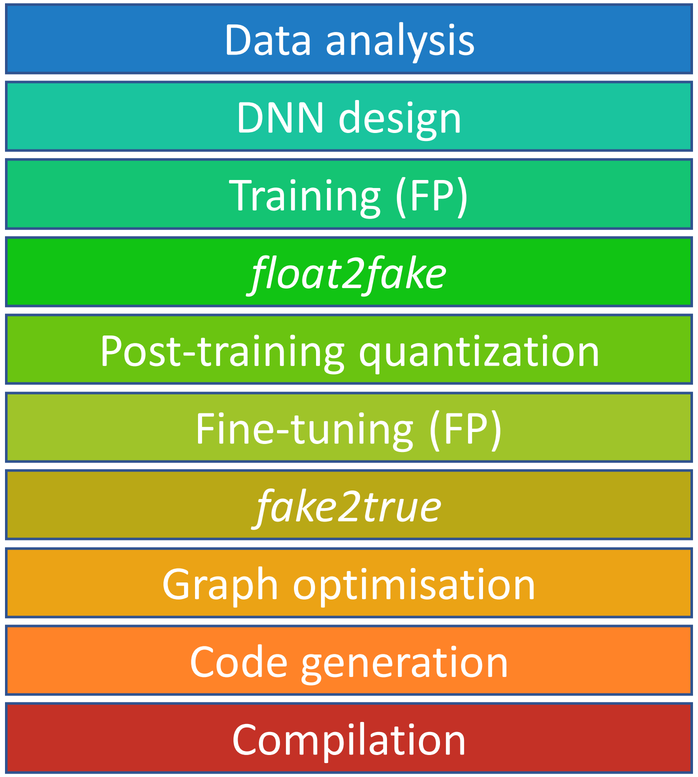


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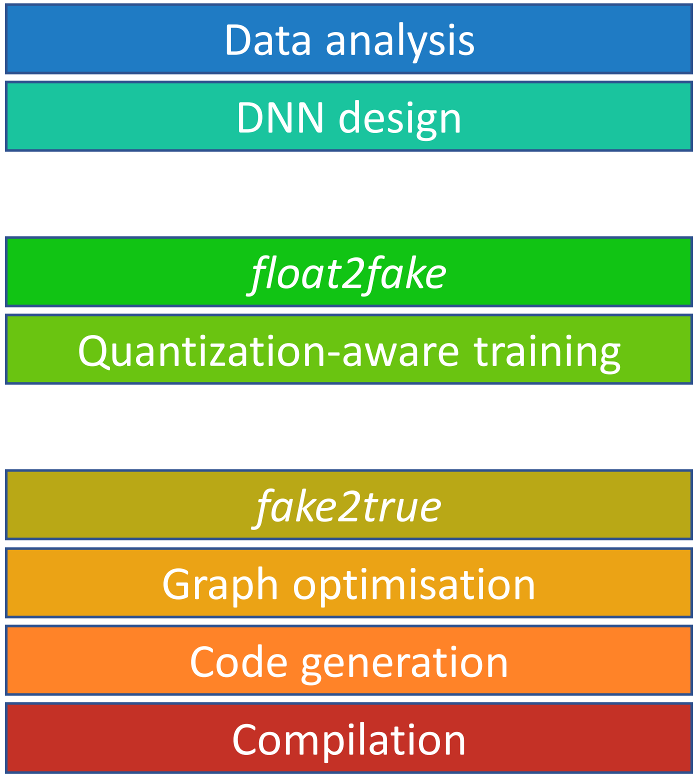


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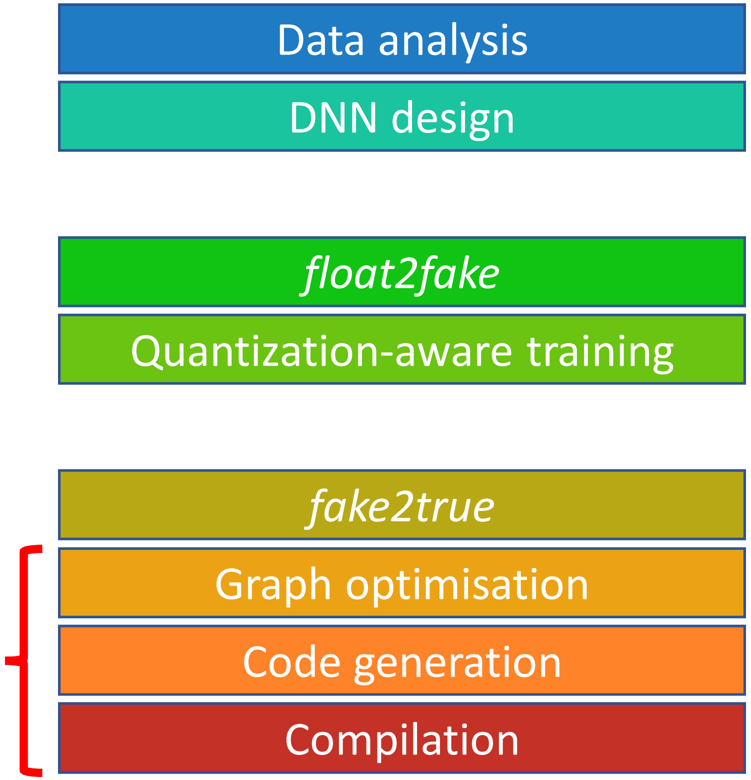


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TODAY WE WILL NOT DEAL WITH THESE STEPS

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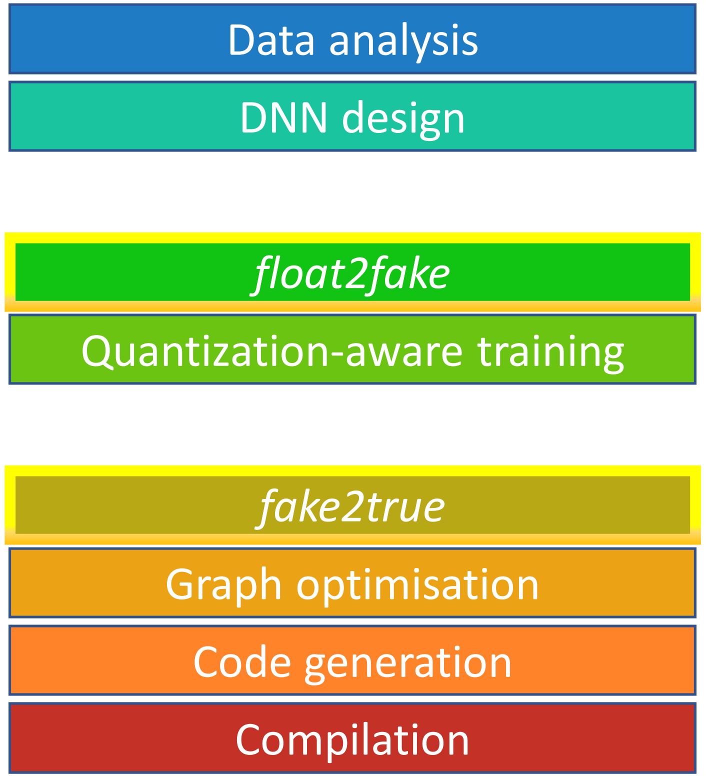


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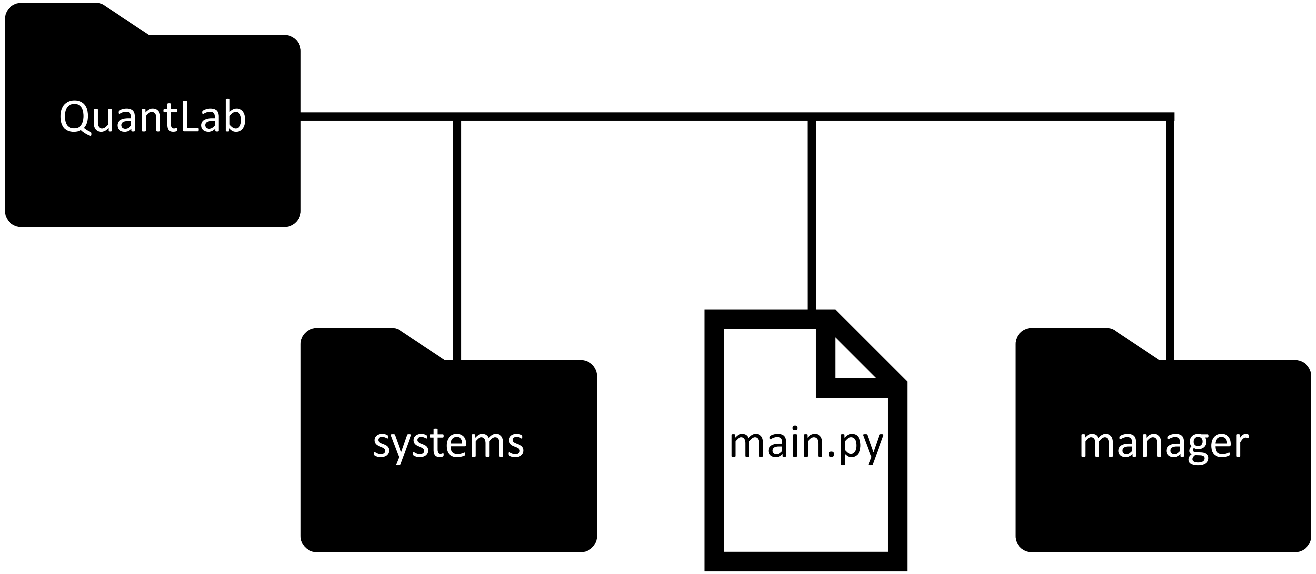

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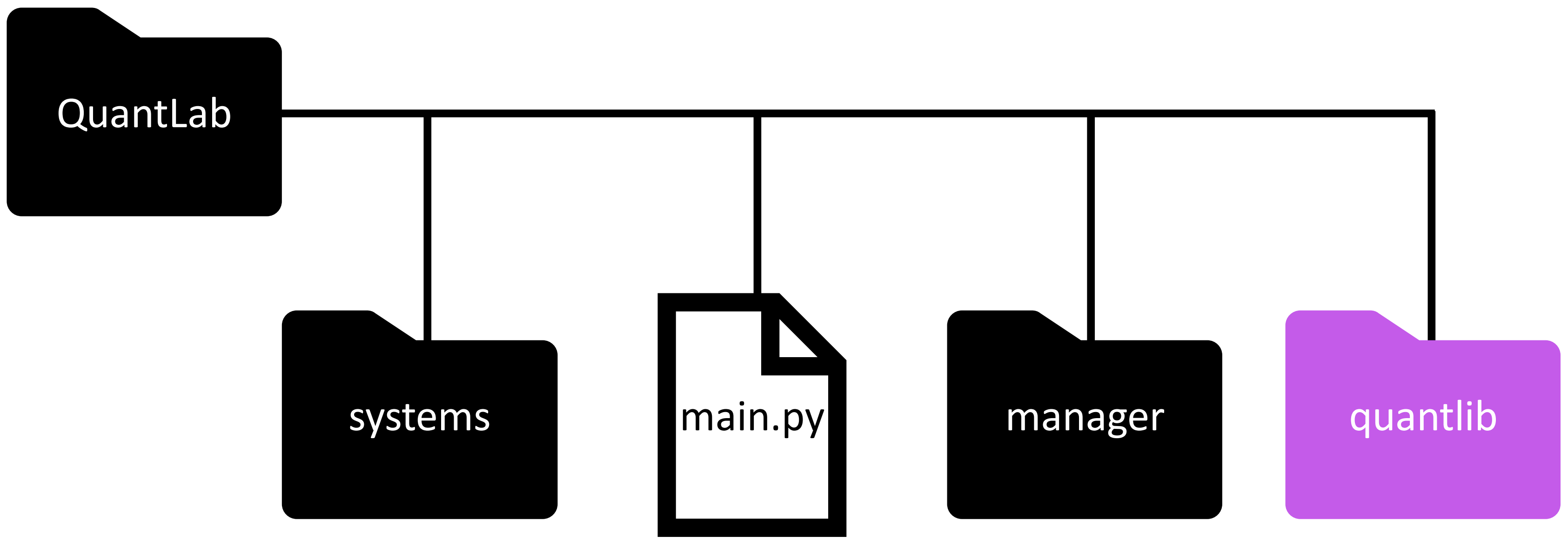
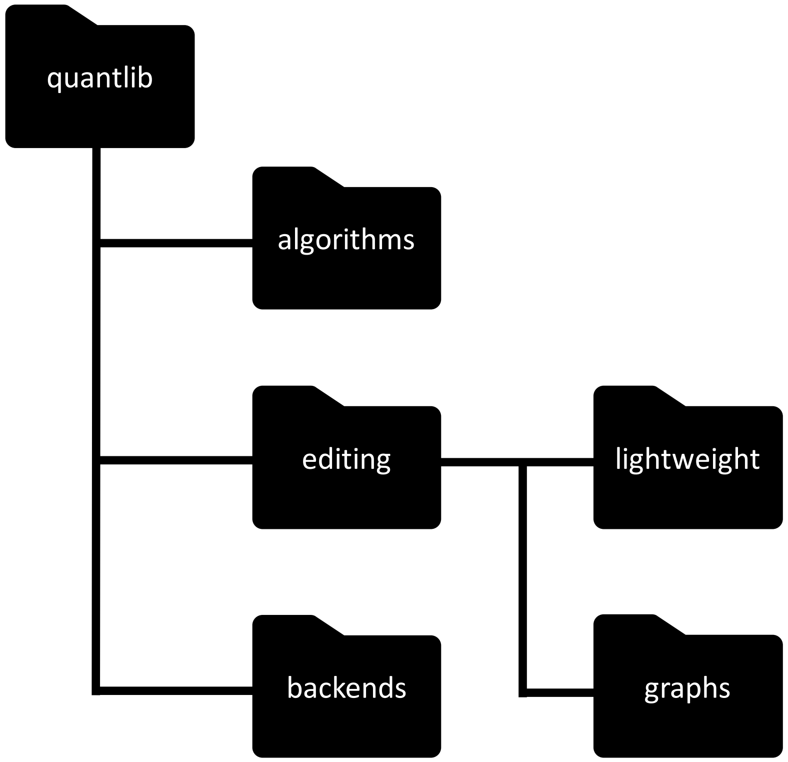


# The `quantlib` package: overview



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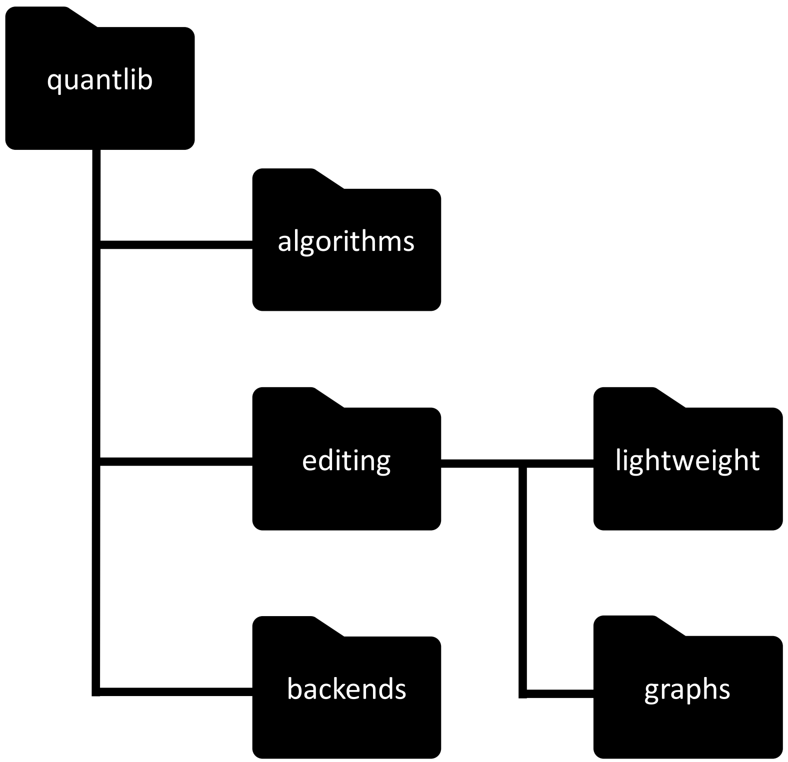


Data analysis

DNN design

*float2fake*

Quantization-aware training

*fake2true*

Graph optimisation

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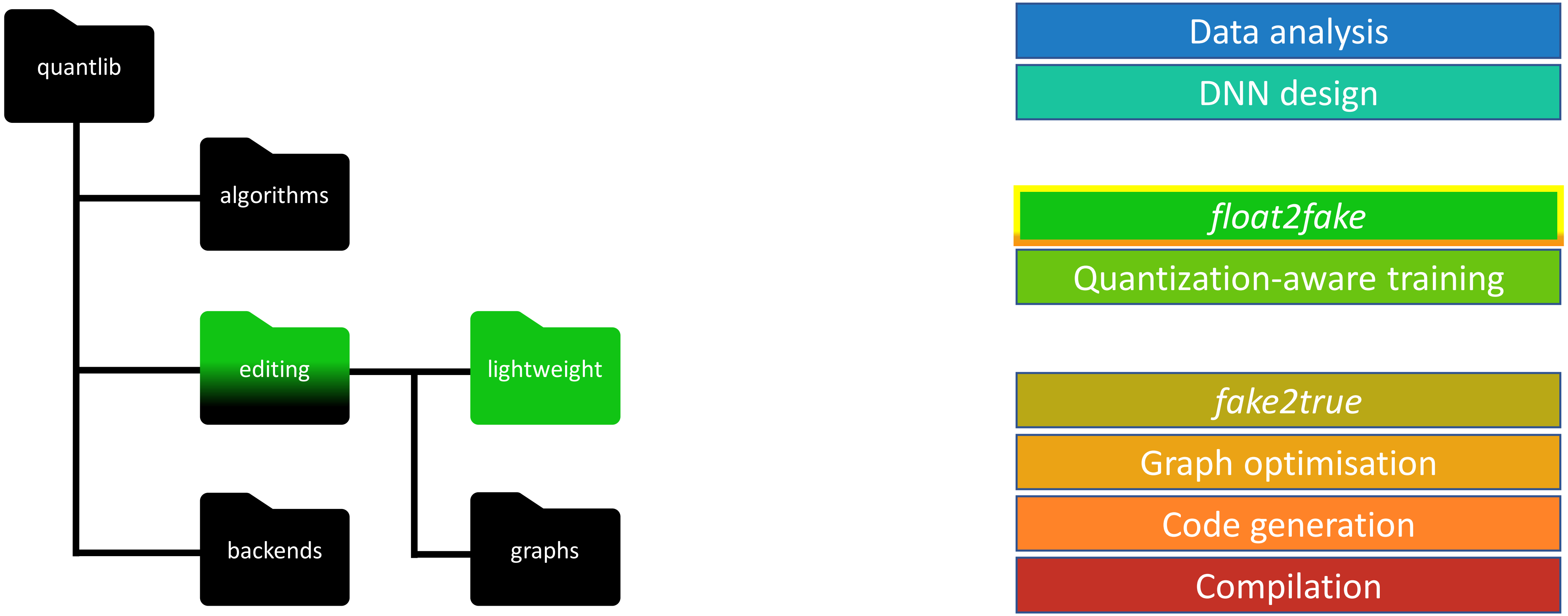

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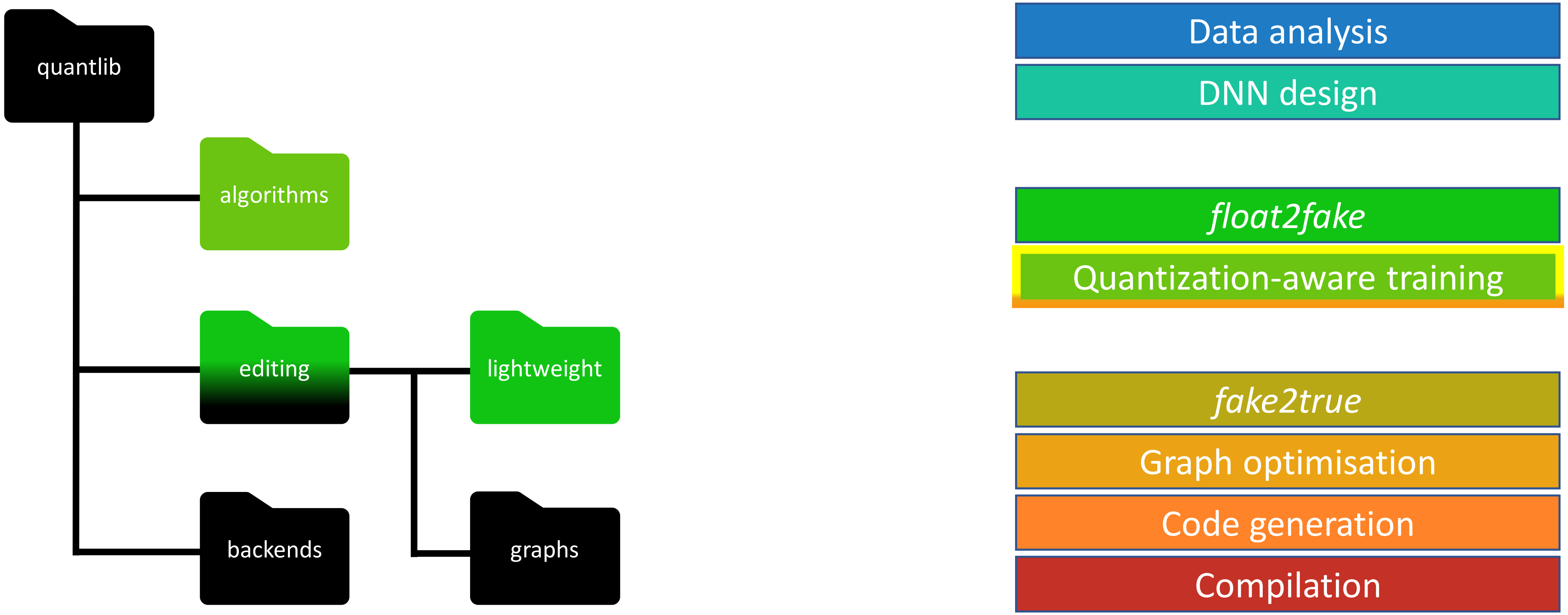

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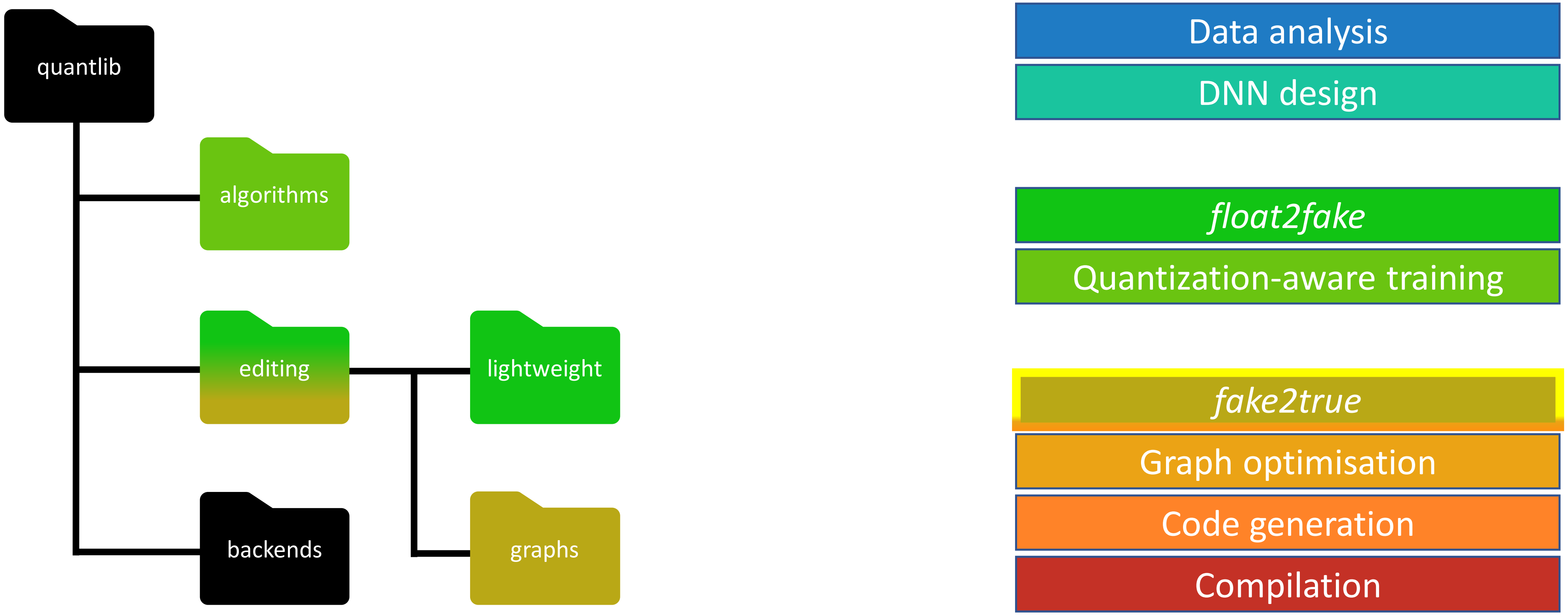

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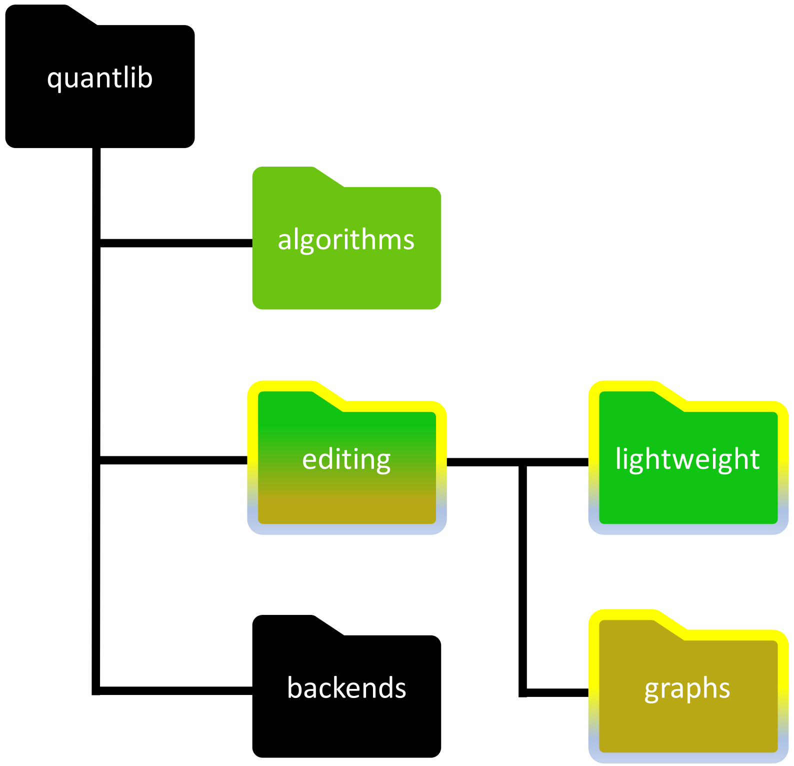


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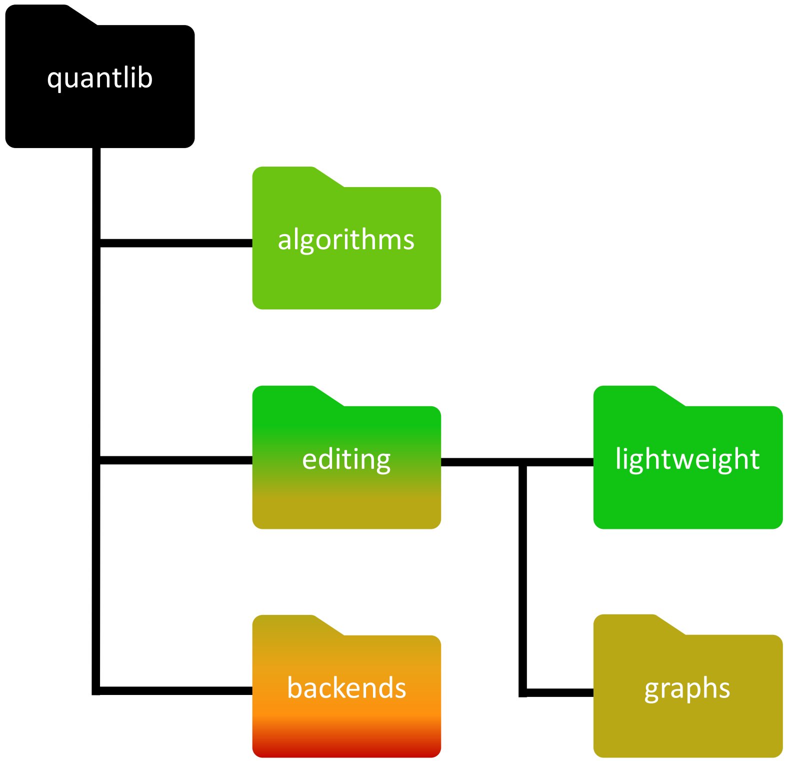
TODAY'S EXERCISES WILL FOCUS ON THESE TOOLS

# The `quantlib` package: overview




Data analysis

DNN design

*float2fake*

Quantization-aware training

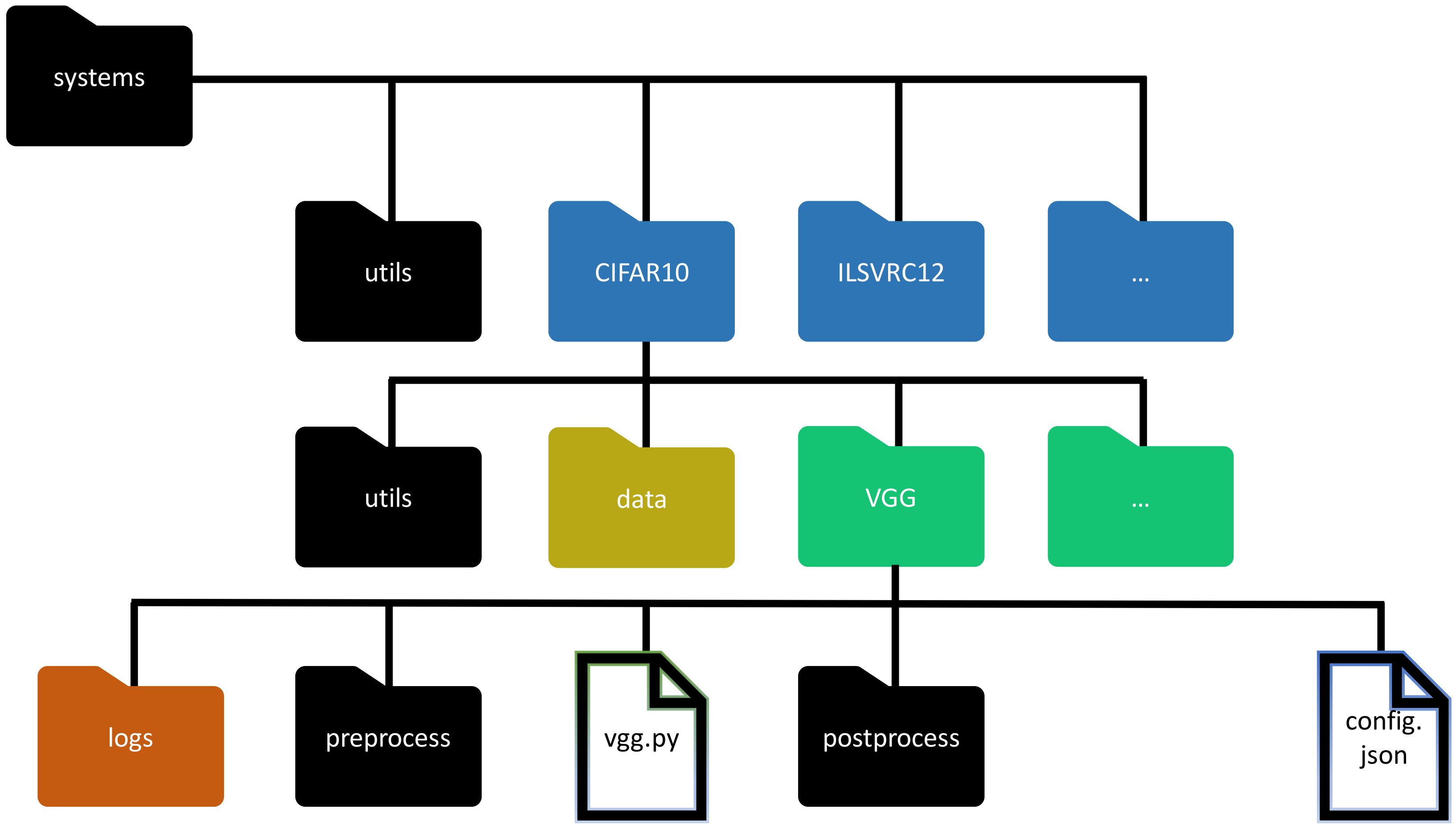
*fake2true*

Graph optimisation

Code generation

Compilation

# Extending topology sub-packages



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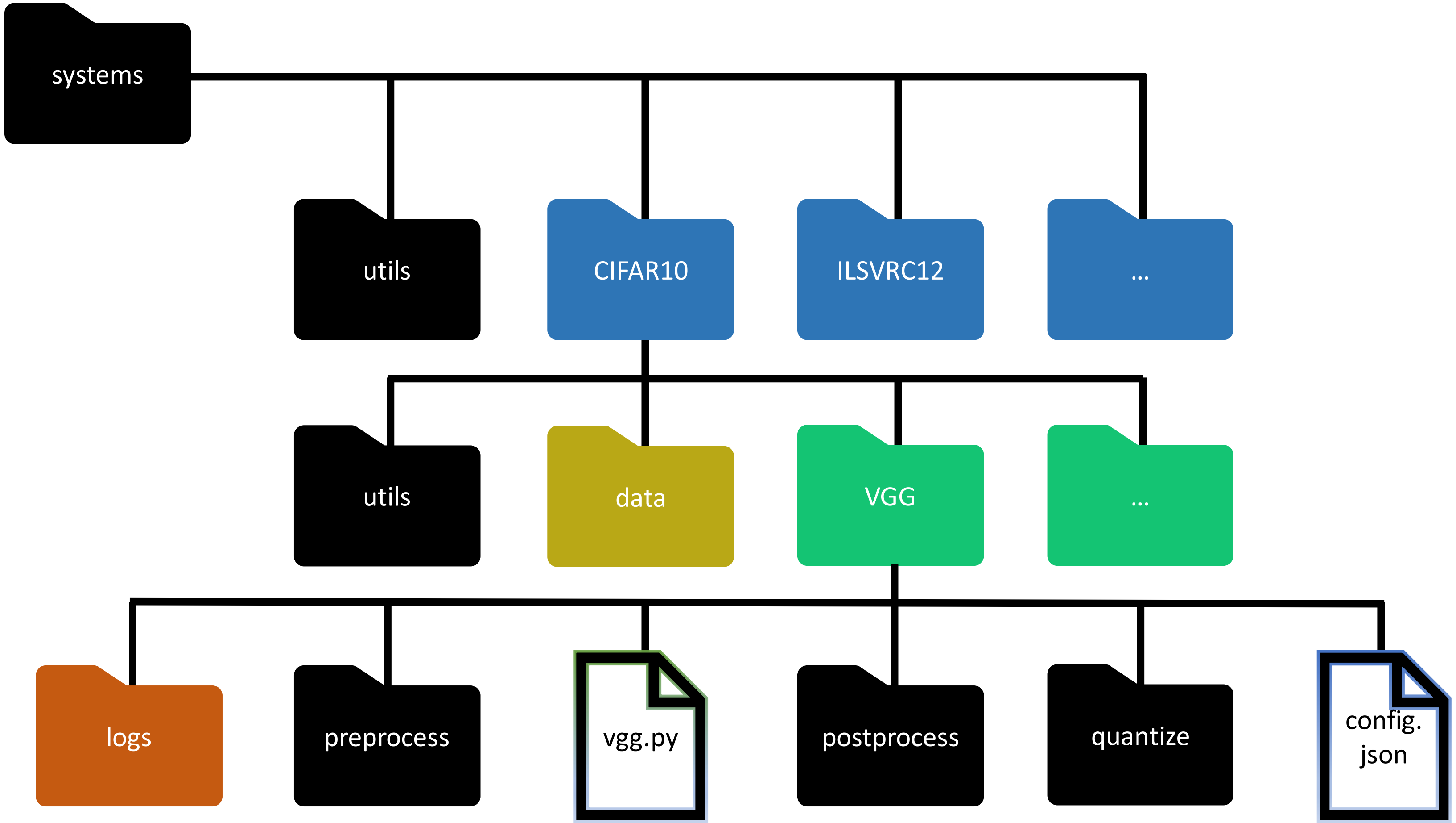

# QuantLab: usage overview

- Create a problem sub-package (remember to prepare the data!)
- Create a topology sub-package
- Write the working files:
    - Data pre-processing and loading
    - Network definition
    - Output post-processing

- Write the configuration file that describes how to instantiate the system
- Run the `configure` flow
- Run the `training` flow

**ITERATE UNTIL YOU ARE SATISFIED!**

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- Create a problem sub-package (remember to prepare the data!)
- Create a topology sub-package
- Write the working files:
  - Data pre-processing and loading
  - Network definition
  - Output post-processing
  - Quantization recipes and network controllers creators (`quantize` namespace)
- Write the configuration file that describes how to instantiate the system
- Run the `configure` flow
- Run the `training` flow
- Perform fake2true conversion
- Generate code for your platform (warning: this is has not been automated yet!)

**ITERATE UNTIL YOU ARE SATISFIED!**

# QuantLab: present and future

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Existing features:

- Configuration-based training flows
- Multi-GPU and multi-process support
- Integration with TensorBoard
- *float2fake* conversion
- Quantization-aware training algorithms (STE, INQ, RPR, ANA, PACT, SAWB)
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Planned features:

- Data and network initialisation seeding
- PyTorch code generation for true-quantized networks
- Post-training quantization
- More quantization-aware training algorithms
- Mixed-precision support

# QuantLab Virtual Workshop

Part 3: graph editing

# Graph editing in `quantlib`

By **graph editing** we refer to a collection of techniques to modify graphs

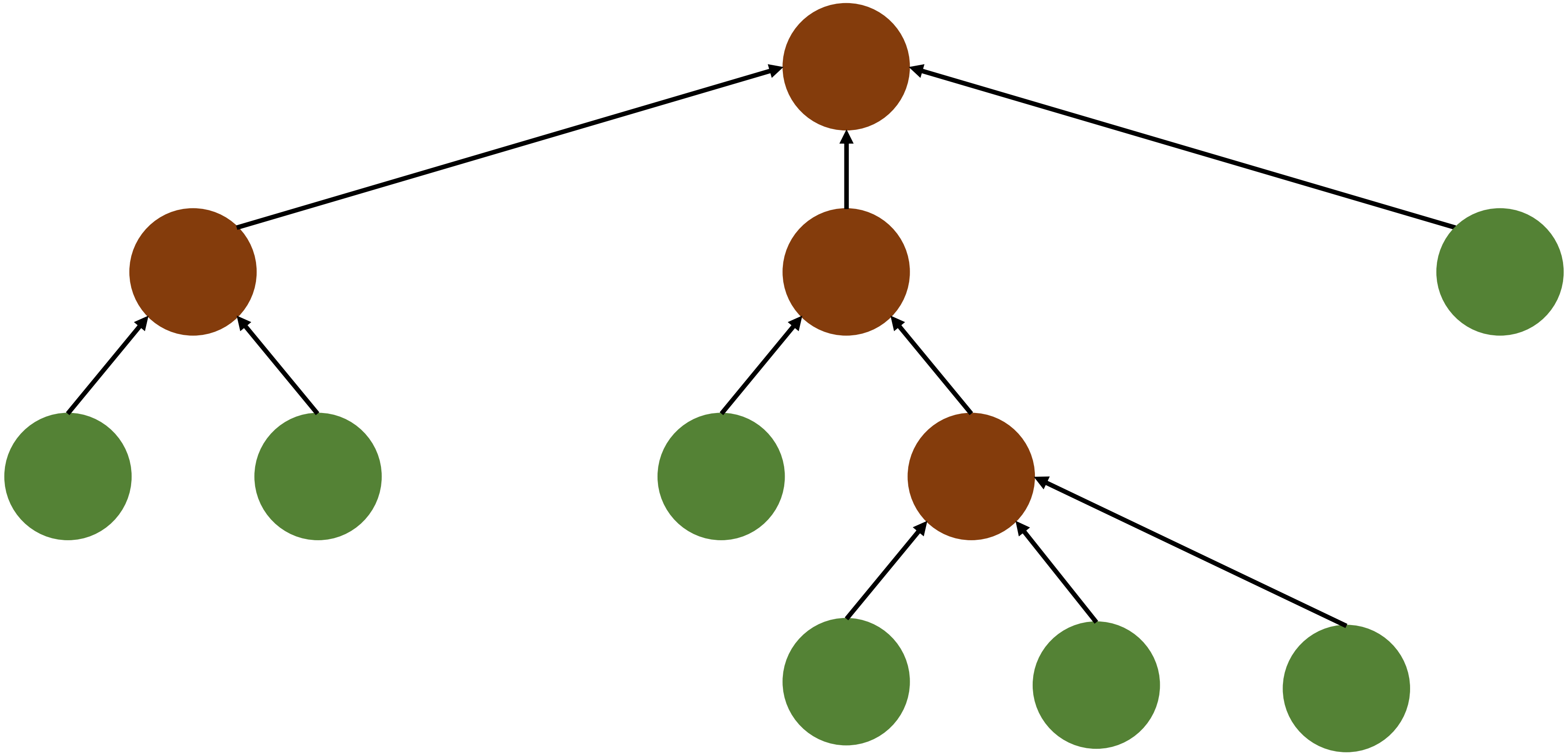
- Tree traversal and leaf replacement
  - *float2fake* conversions

- Graph morphisms and algebraic graph rewriting
  - *fake2true* conversions

# Tree traversal and leaf replacement

- **Tree**: a directed graph G whose associated undirected version is connected and acyclic
- **Rooted tree**: a tree where a node has been designated to be the *root*; nodes with no incoming edges are called *leaves* (we assume that the natural orientation of arcs is towards the root)
- **Tree traversal**: the process by which, starting from the root of a rooted tree, all leaves are identified
- **Leaf replacement**: the process by which a leaf is replaced by another leaf, or by a rooted tree whose root takes the place of the leaf

# Tree traversal and leaf replacement



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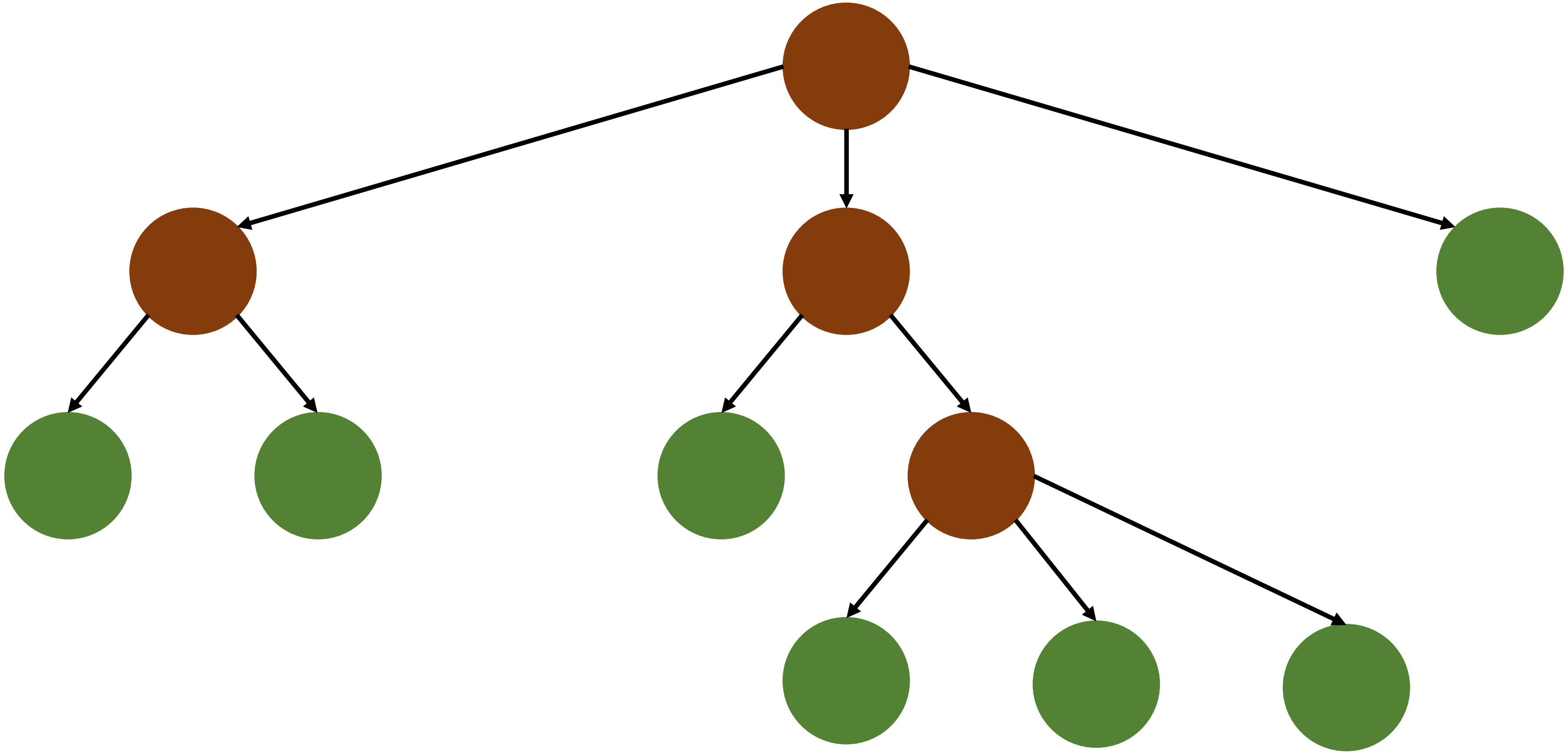

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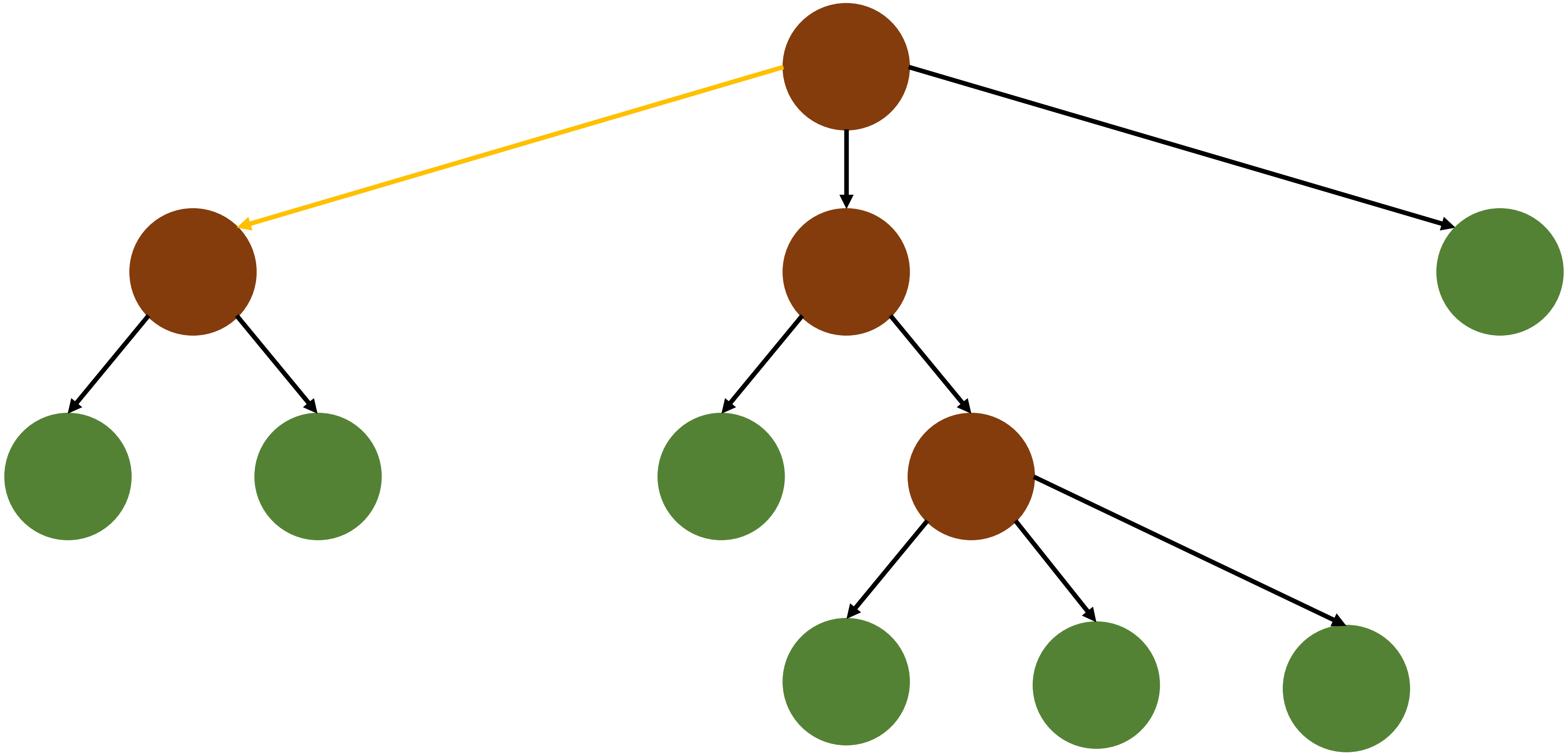

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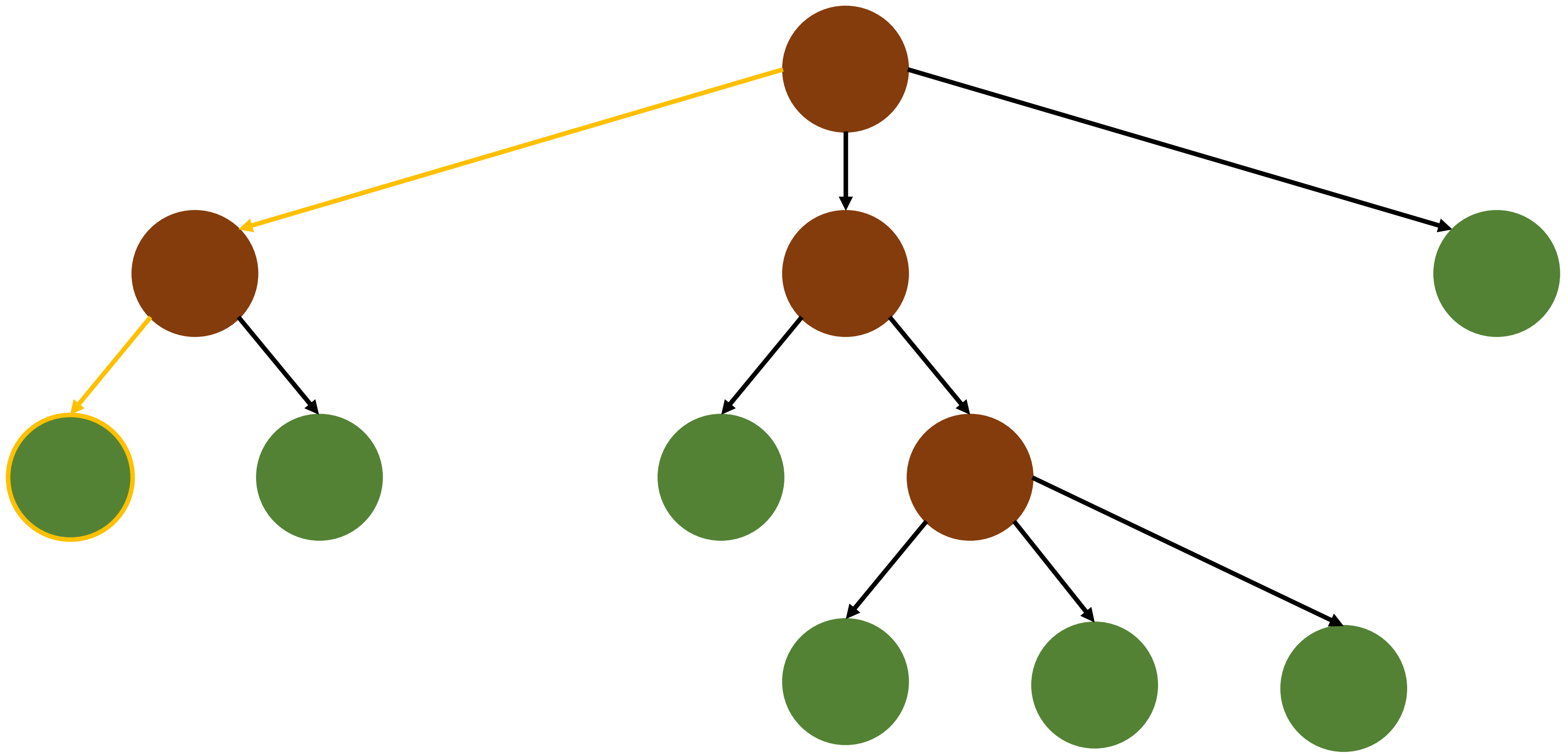

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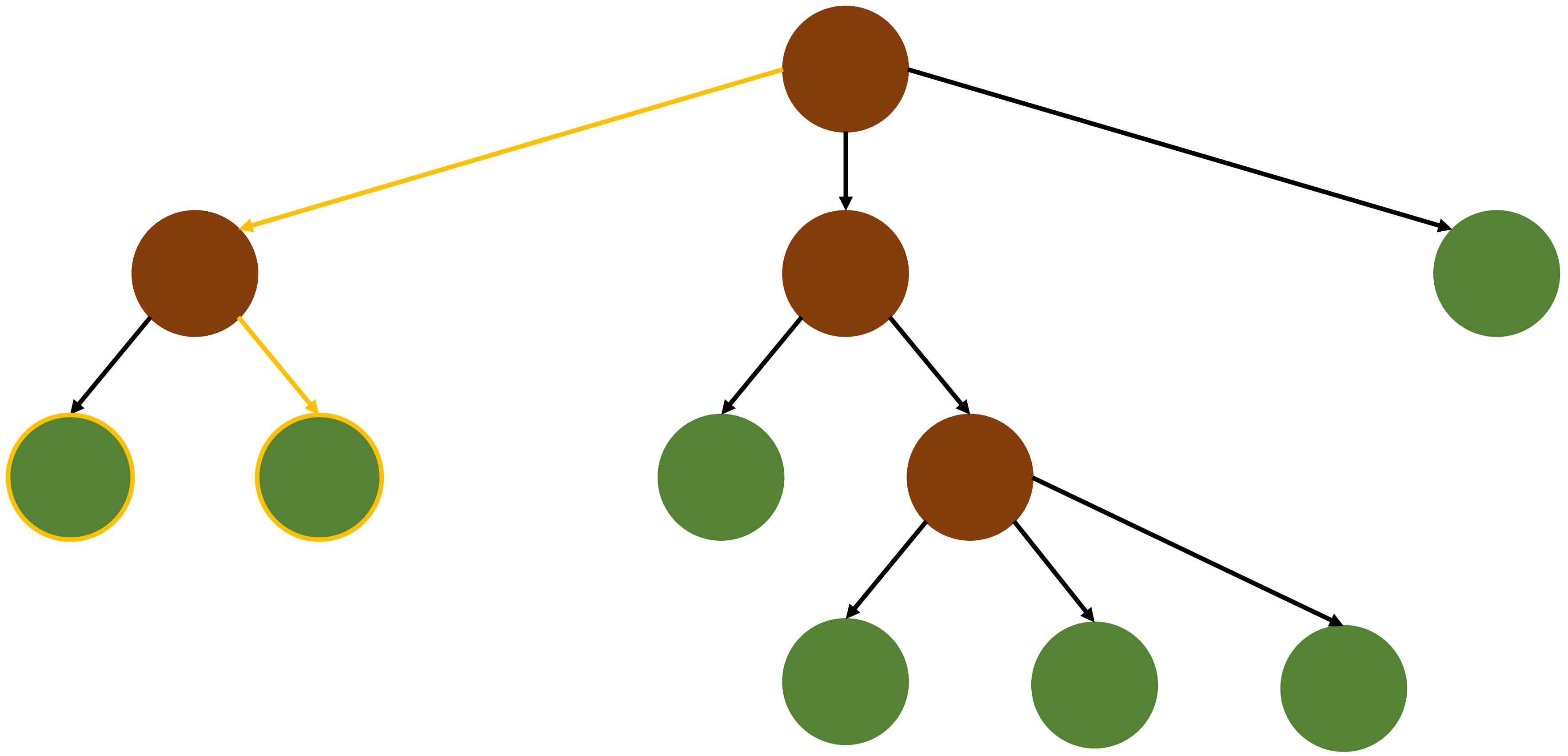

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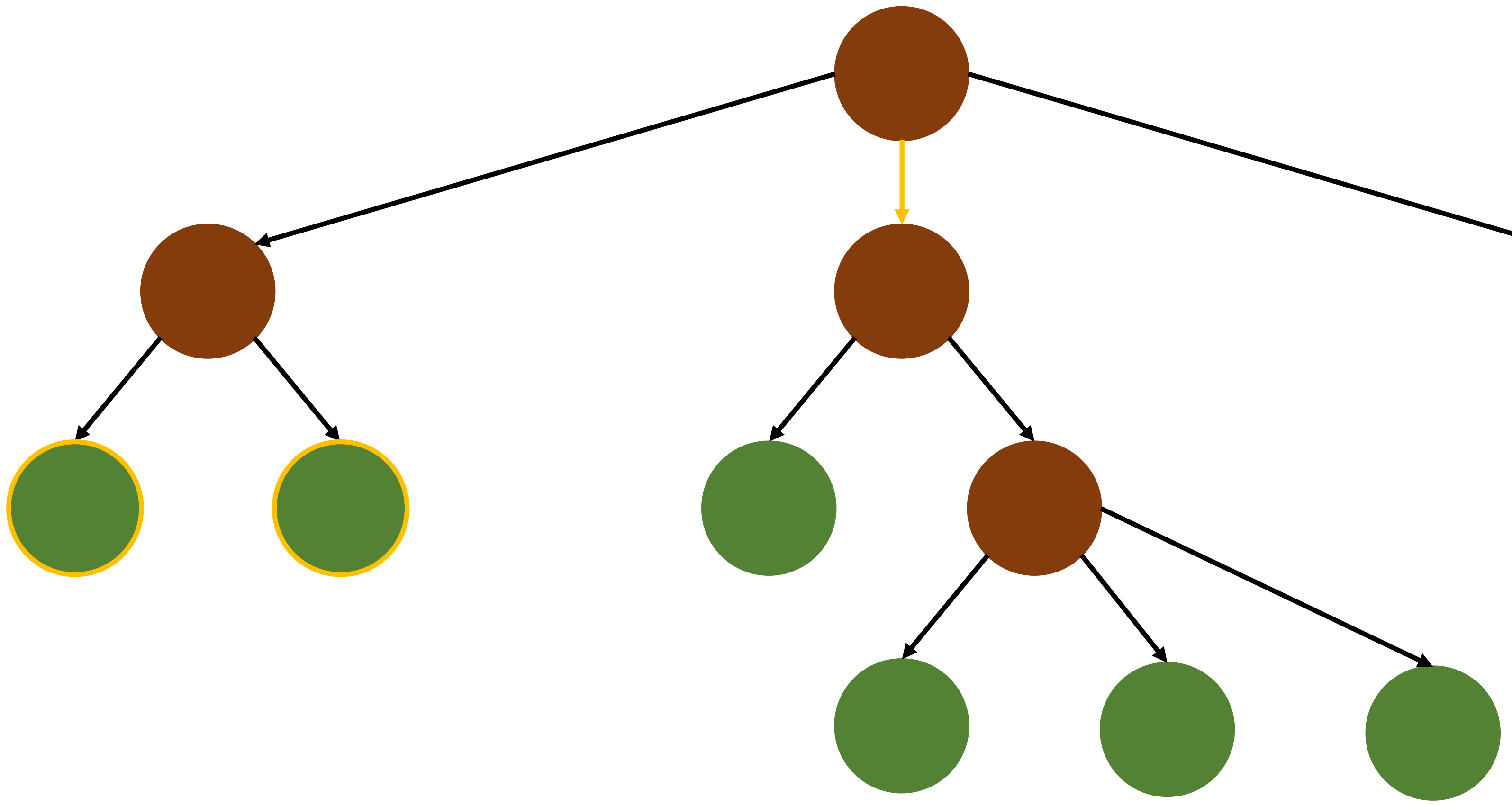

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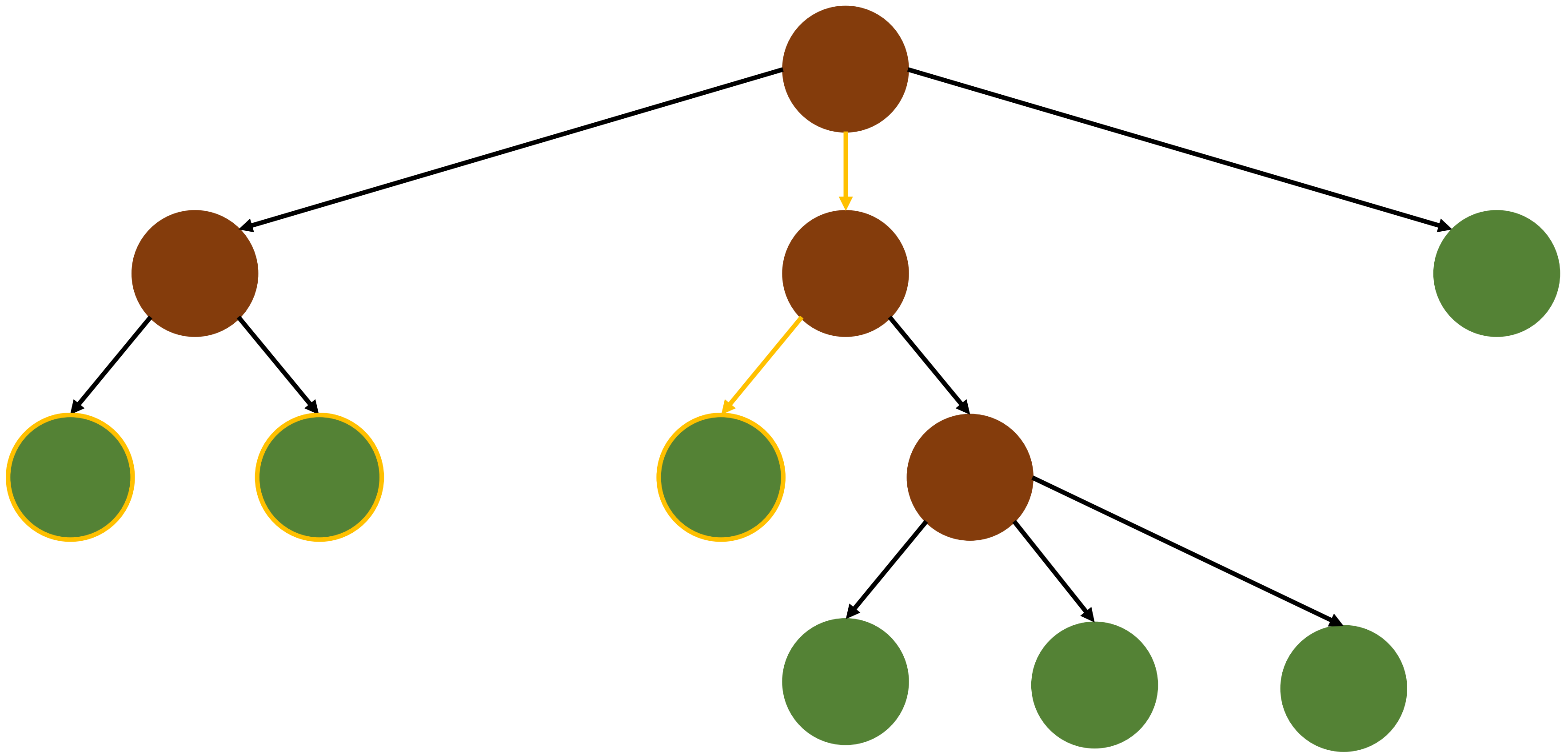

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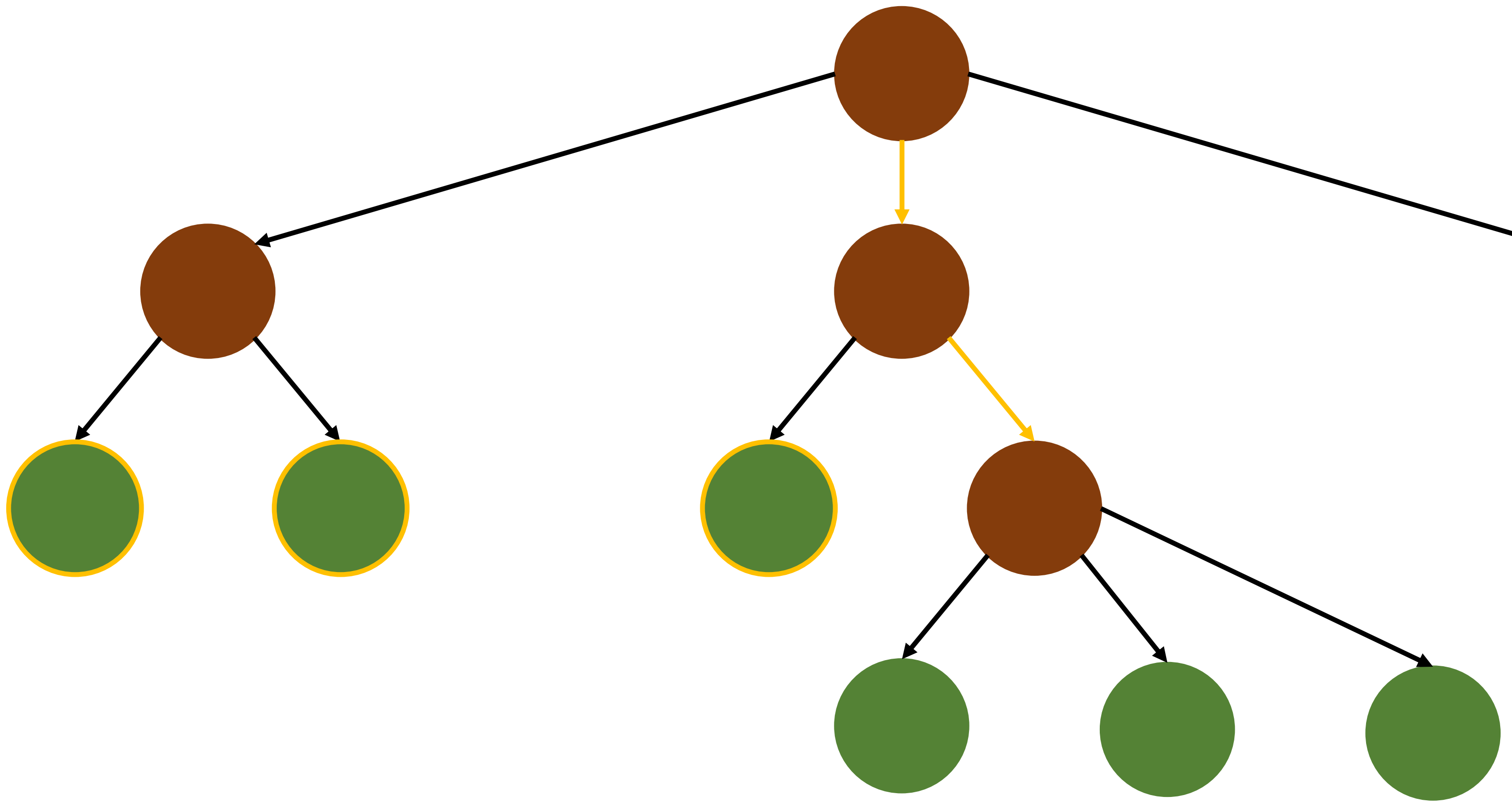

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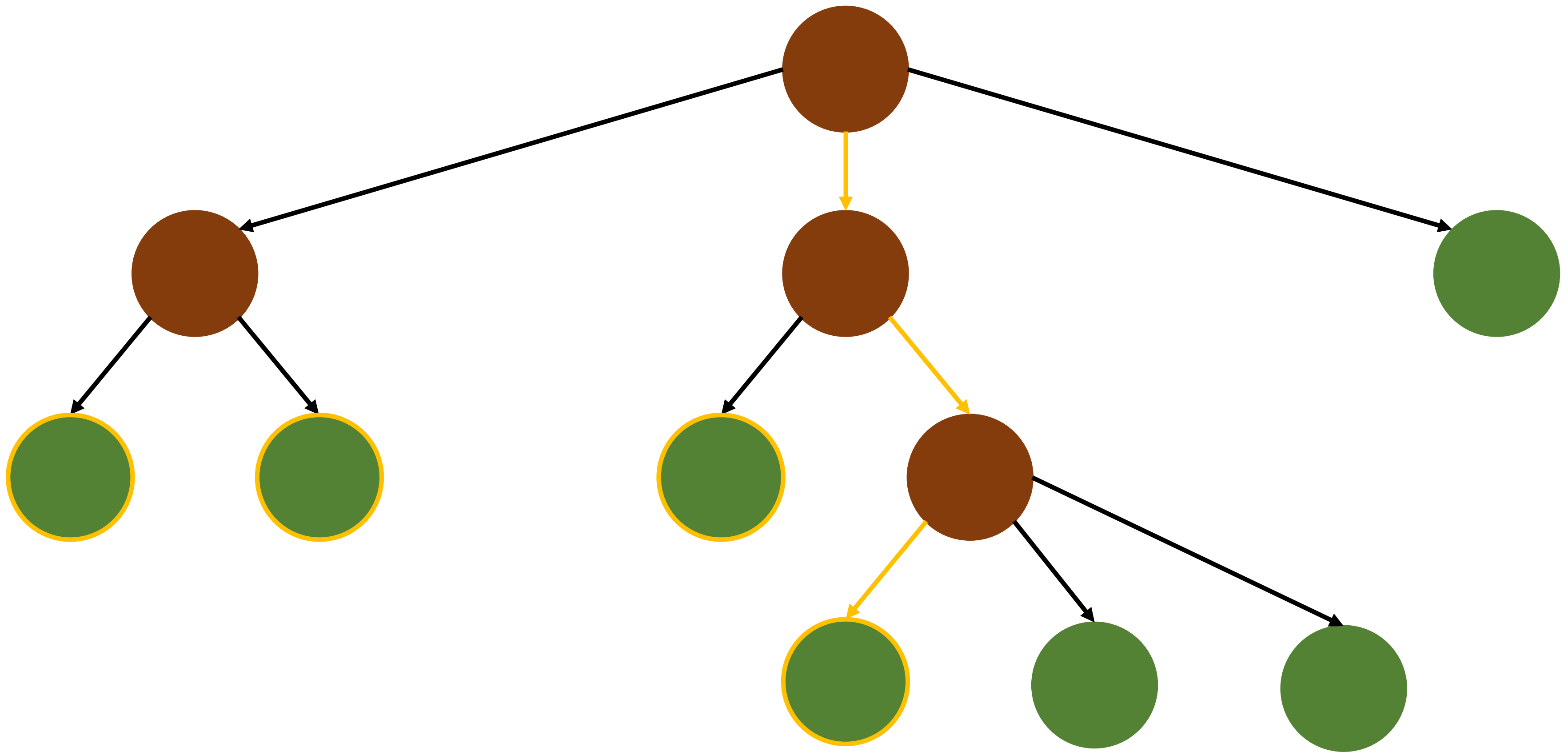

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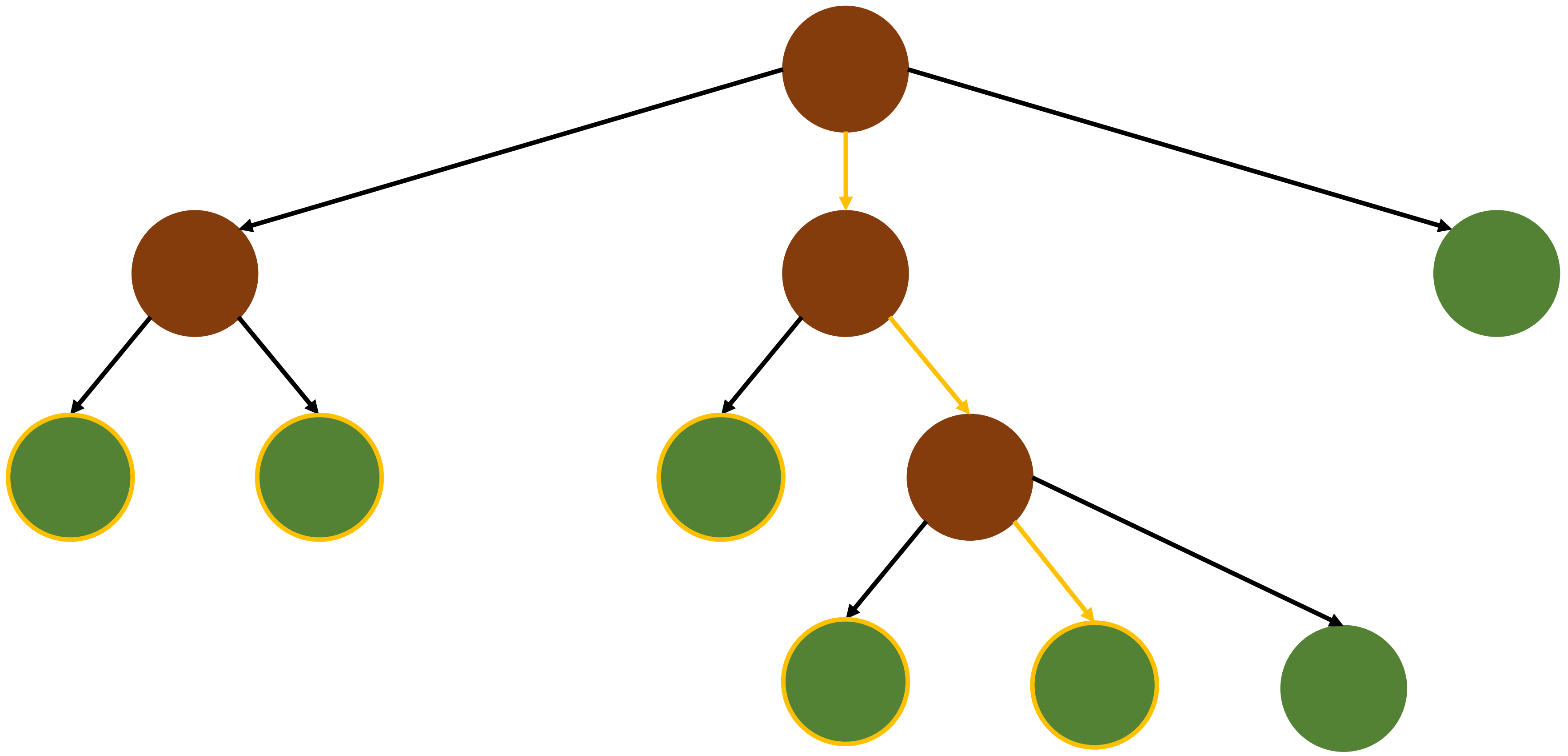

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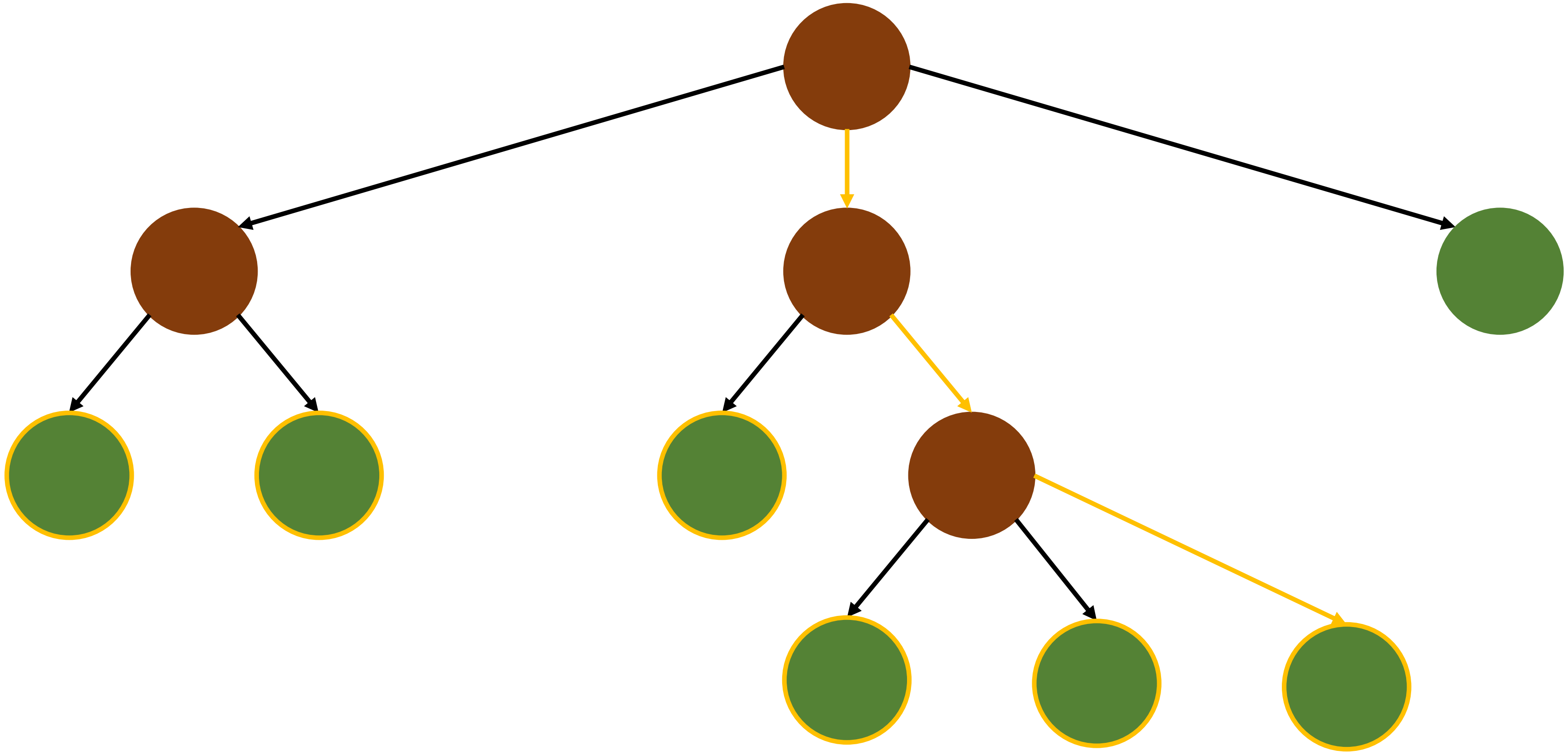

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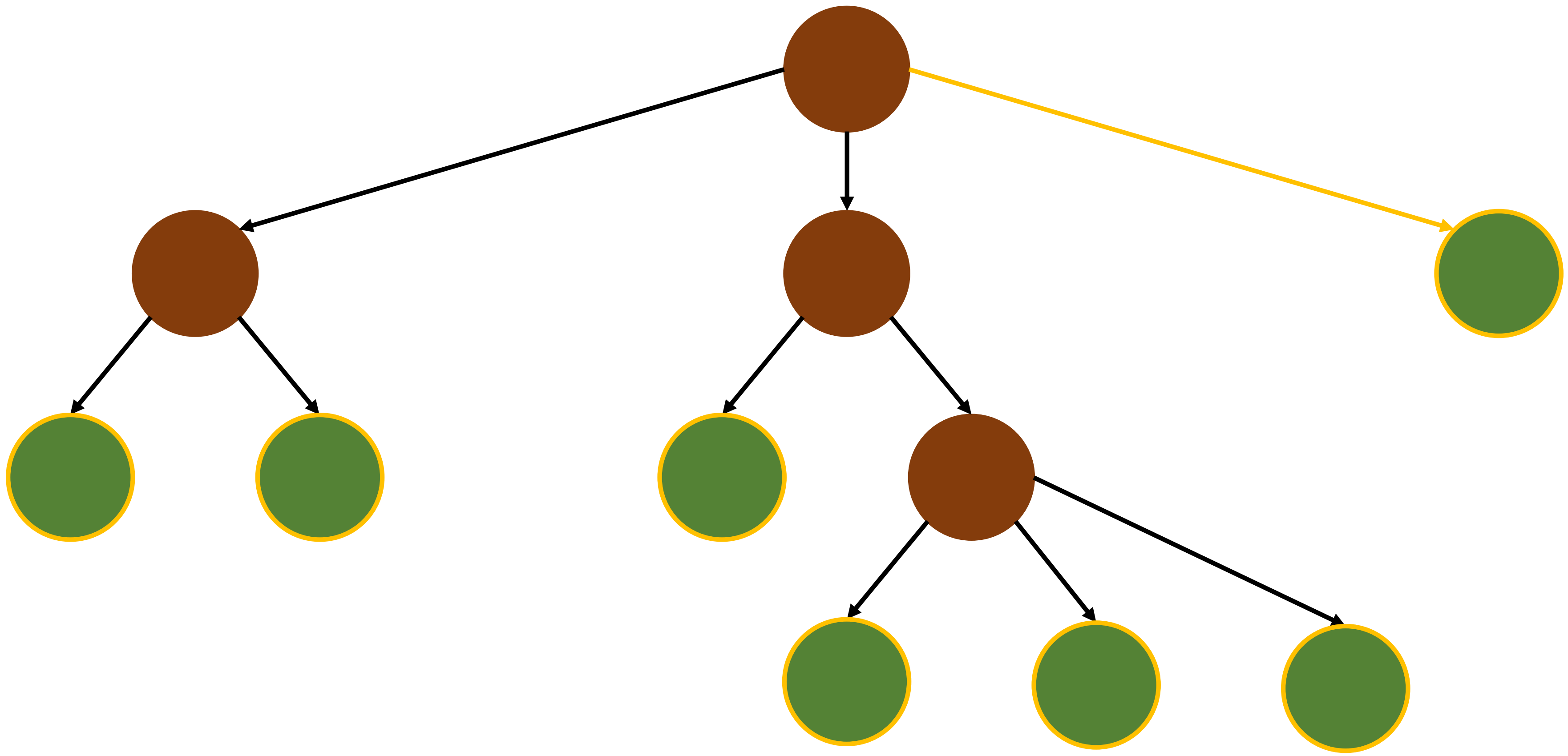

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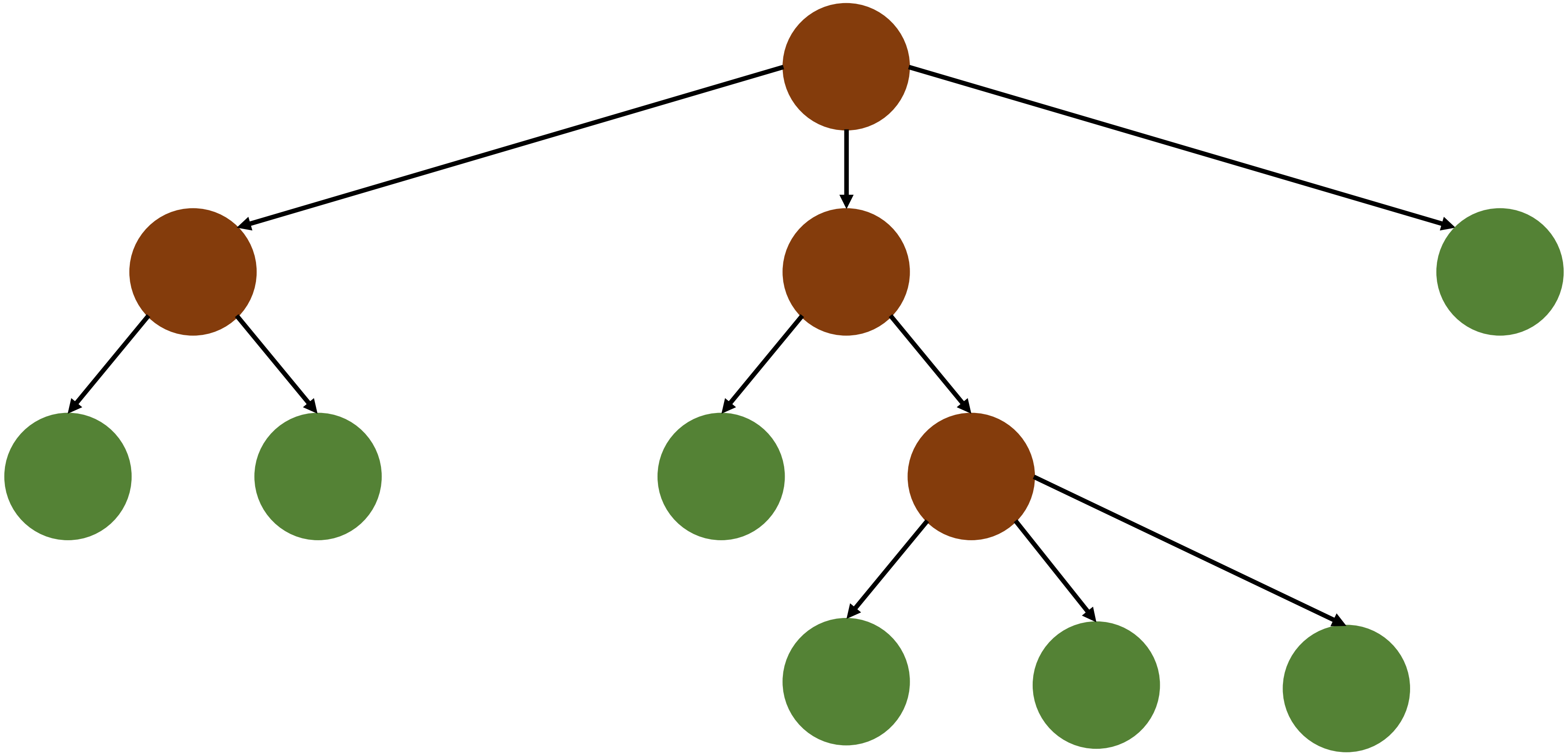

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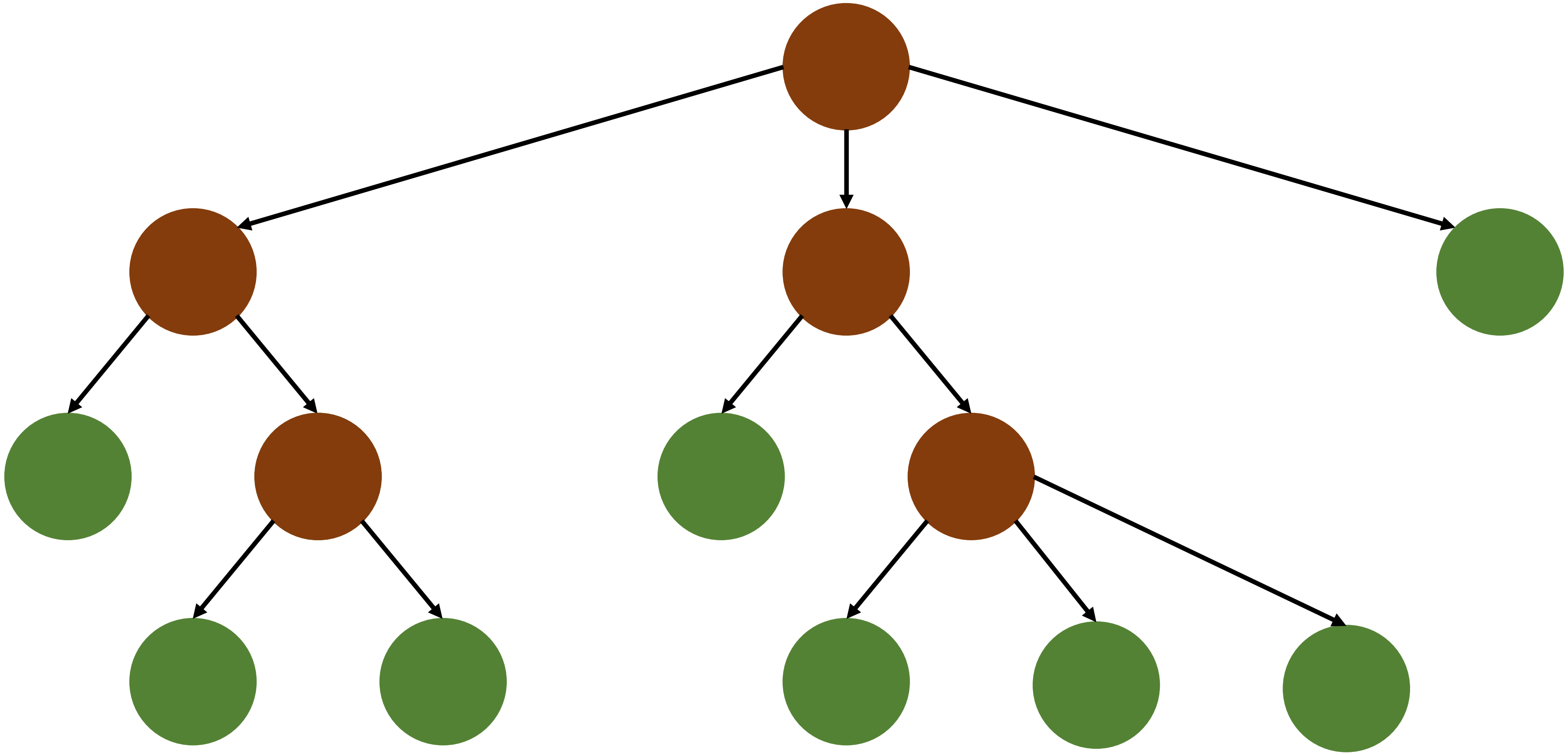


# Graph terminology - advanced

- **Source** and **target** of an arc:
  - $s_G : E \to V,\ s_G\big((u,v)\big) := u$
  - $e_G : E \to V,\ s_G\big((u,v)\big) := v$

- Let $\Lambda \neq \emptyset$ denote a set of **labels**
- Let $* \in \Lambda$ denote an *undefined* label
- **Attributed graphs**
  - Node labelling $l_G : V \to \Lambda$
  - Arc labelling $m_G : E \to \Lambda$

# Functions between graphs

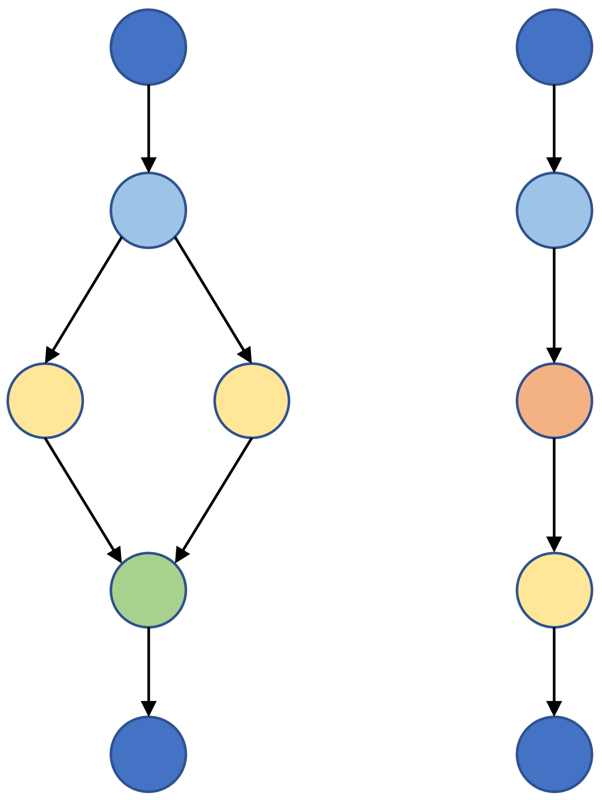
- Let $L = (V_L, E_L), H = (V_H, E_H)$ be graphs
- Since a graph is a pair of sets, a *function between graphs* $L, H$ is a pair $g = (g_V, g_E)$ of functions
  - $g_V : V_L \to V_H$
  - $g_E : E_L \to E_H$

# Preserving the information flow: morphisms

- Preserve the *structural* flow:
  1. $s_H\big(g_E(e)\big) = g_V\big(s_L(e)\big), \forall e \in E_L$
  2. $t_H\big(g_E(e)\big) = g_V\big(t_L(e)\big), \forall e \in E_L$
- Preserve the *semantic* flow:
  3. $l_H\big(g_V(v)\big) = l_L(v), \forall v \in V_L$
  4. $m_H\big(g_E(e)\big) = m_L(e), \forall e \in E_L$
- A function between graphs $L, H$ that satisfies $1., 2., 3., 4.$ is called a **morphism**
- Can you think of a function between graphs which is not a morphism?

# Algebraic graph rewriting

- **Graph rewriting rule:**
  - Context graph
  - Template graph and template core
  - Replacement graph and replacement core
- **Derivation**: recursive definition: application or sequence of derivations
- **Application point**: a morphism; in practice we use type-checked isomorphisms



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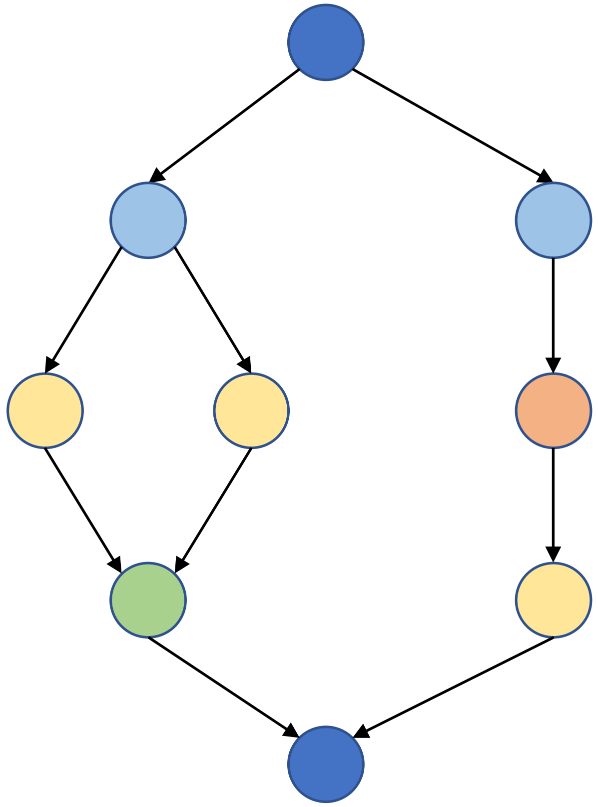

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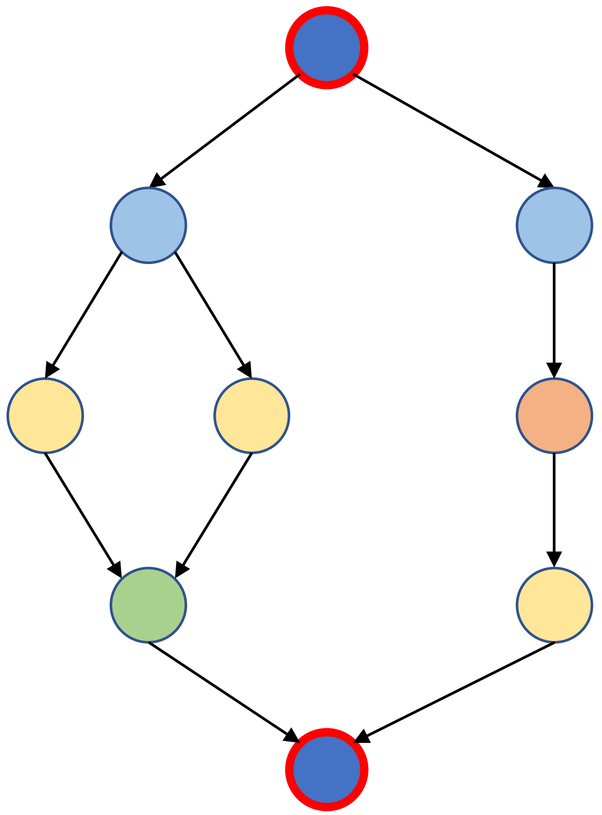

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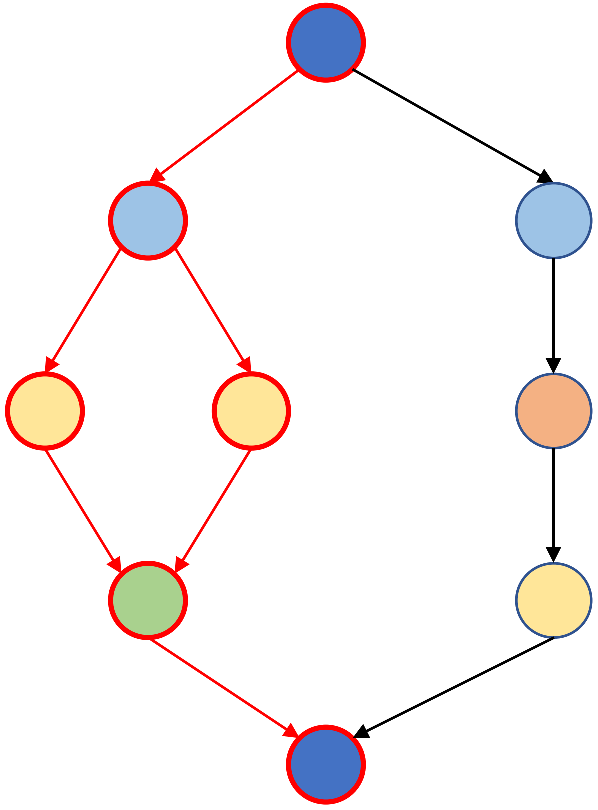

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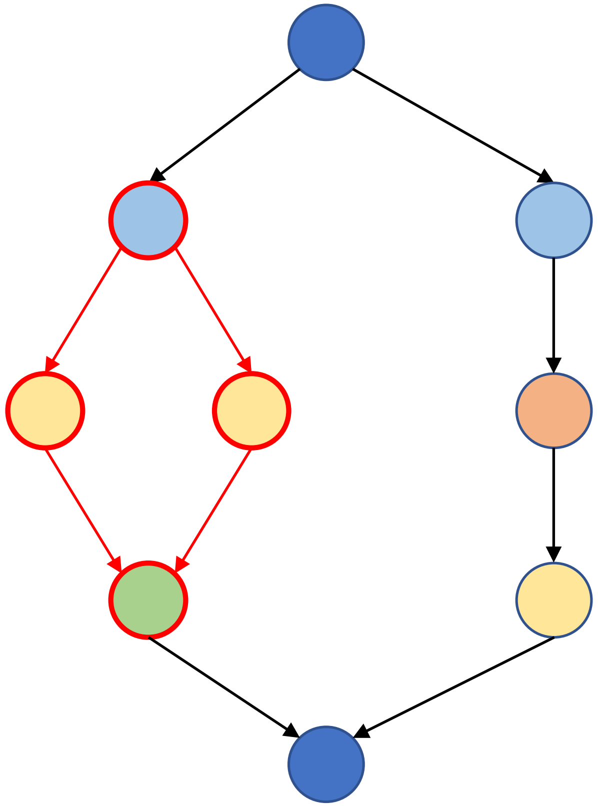

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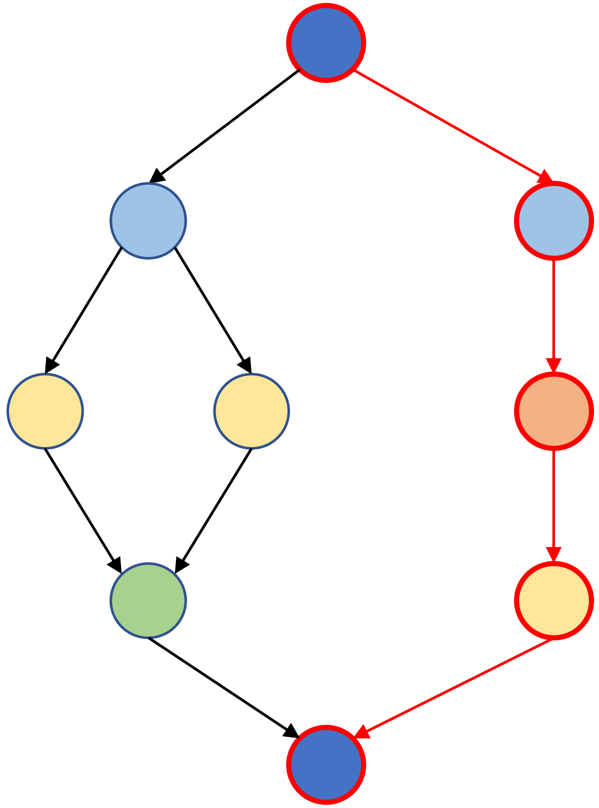

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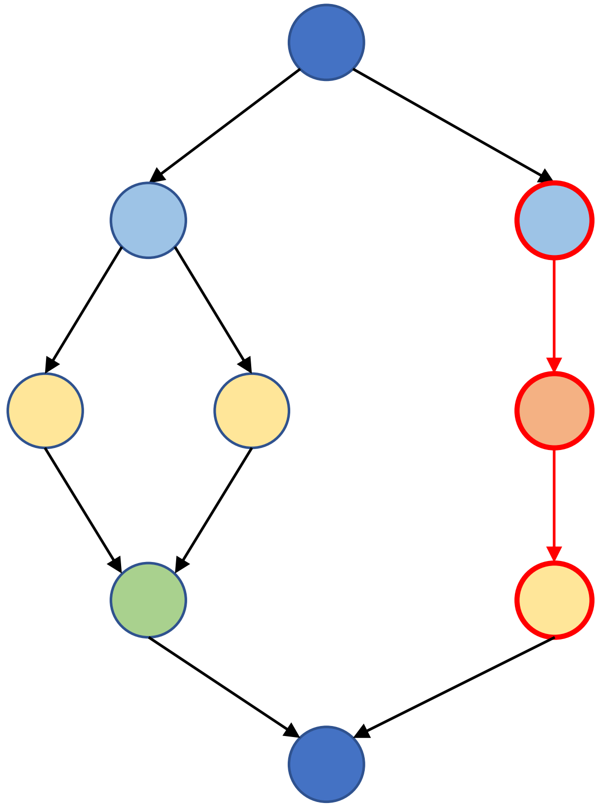
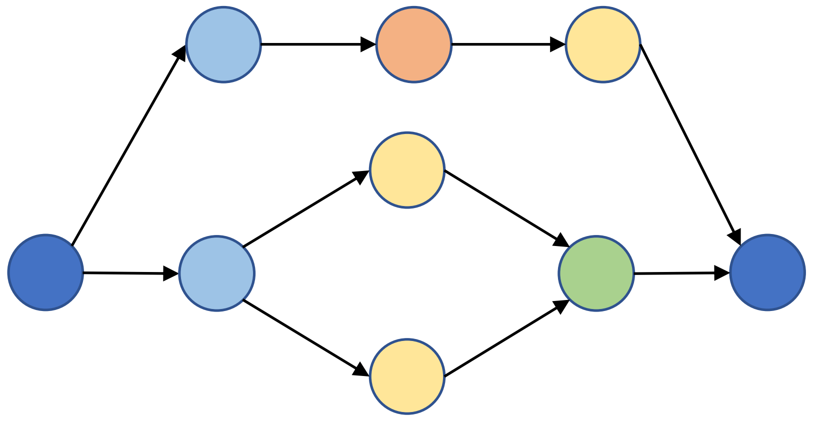
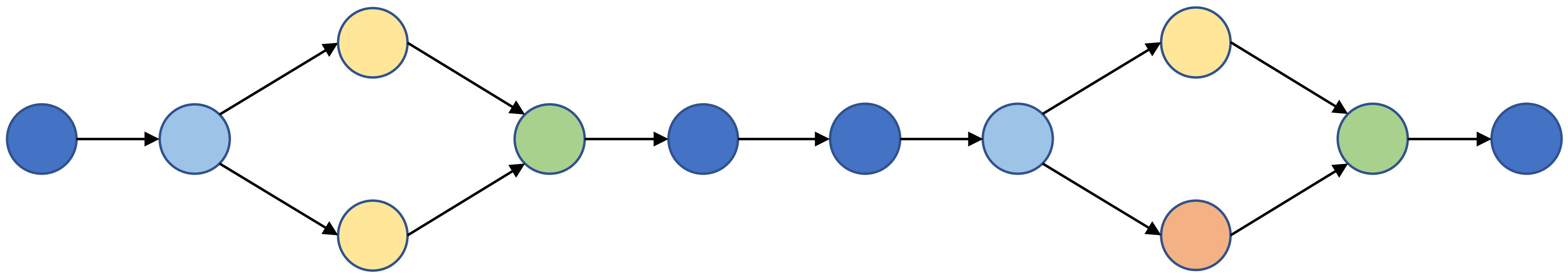
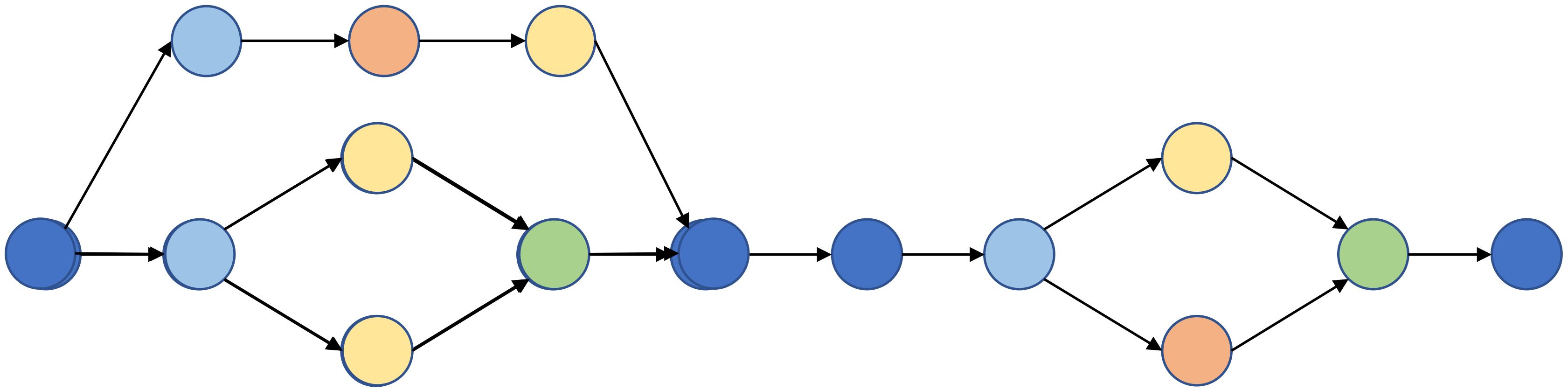
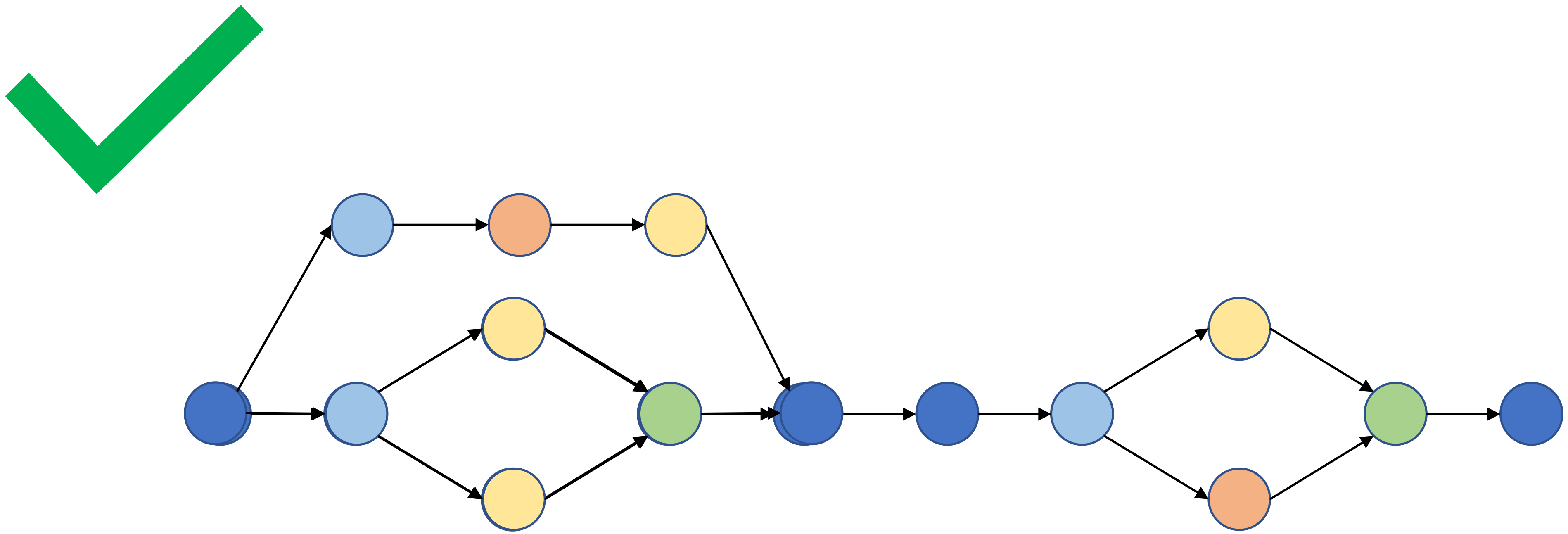
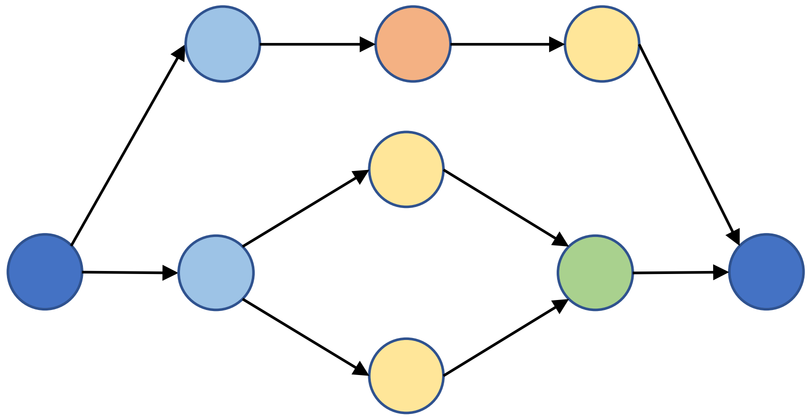


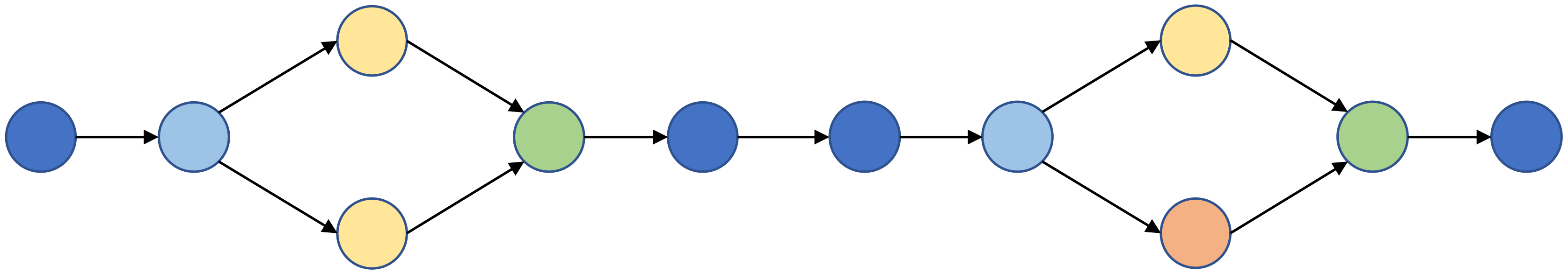


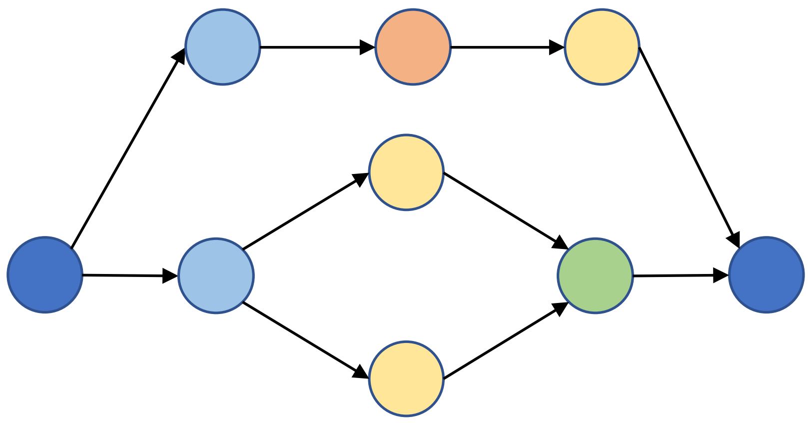


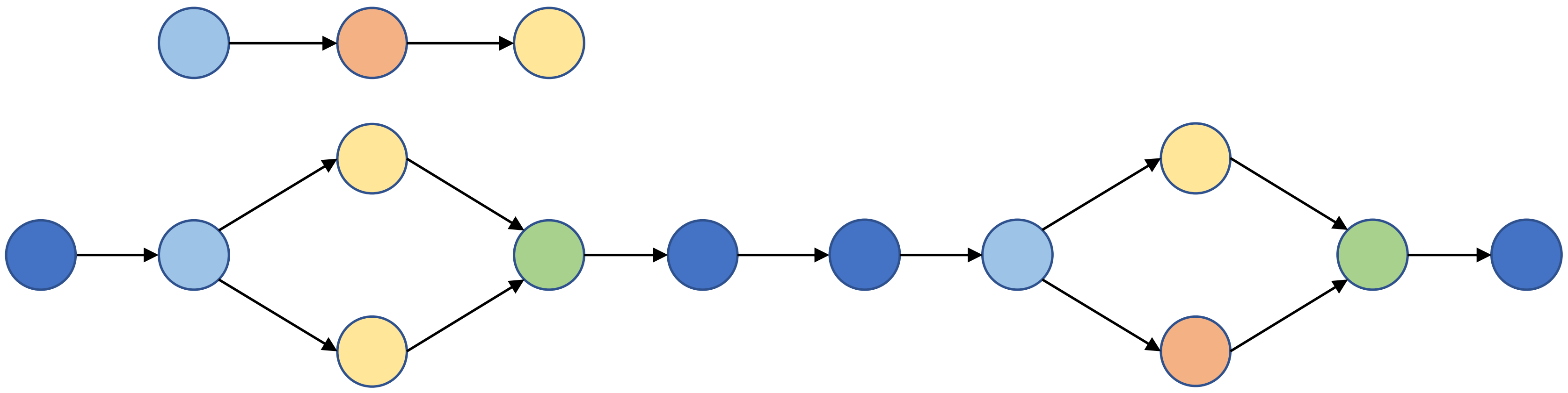


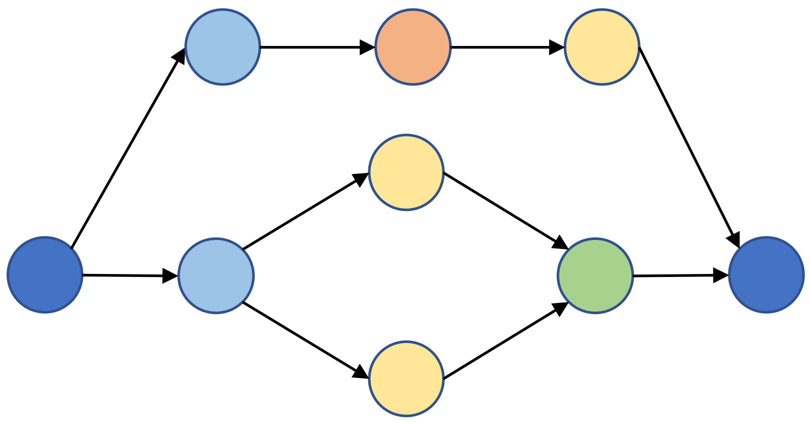


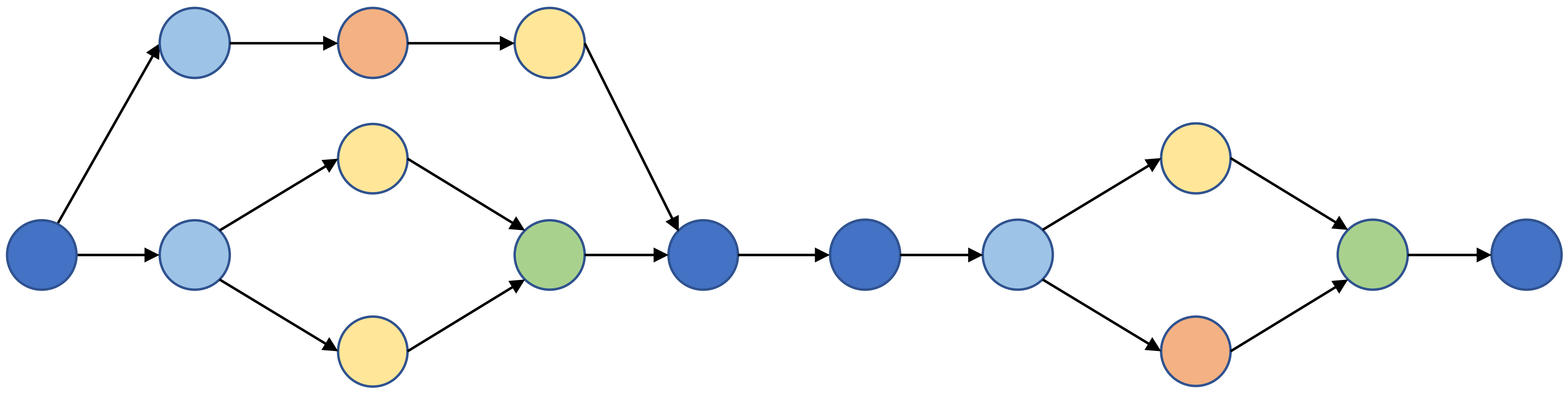


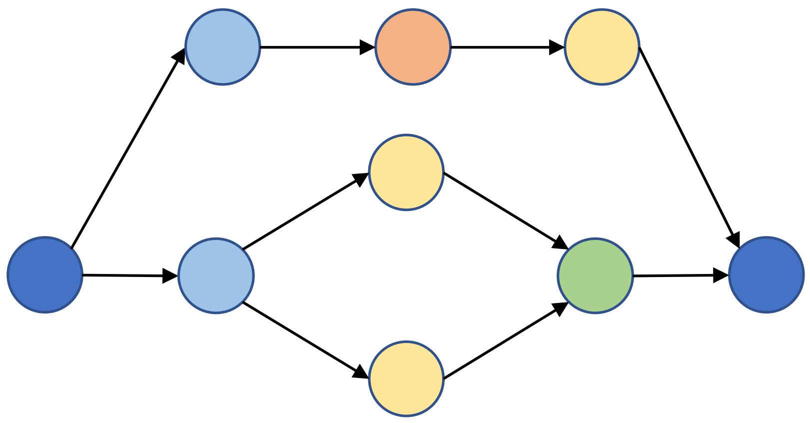


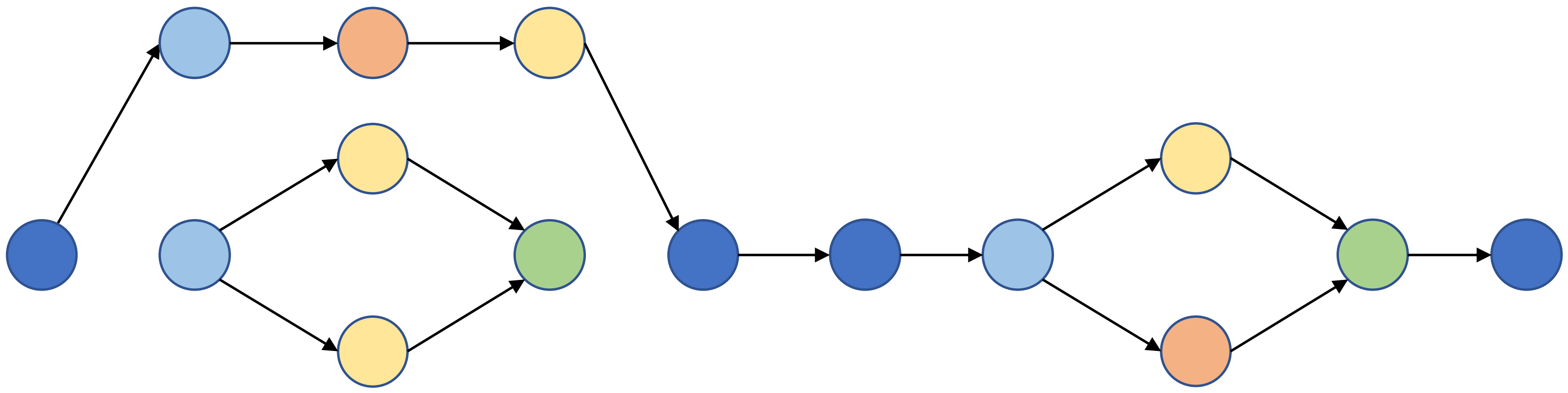


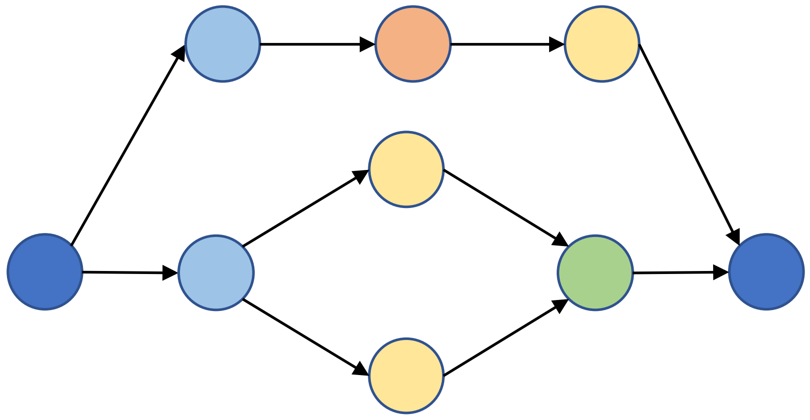


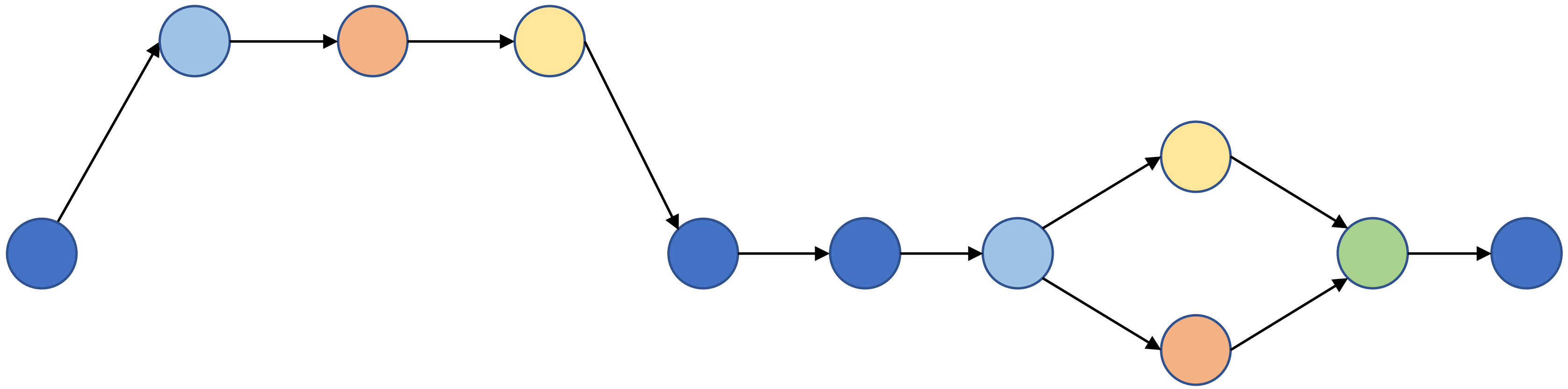


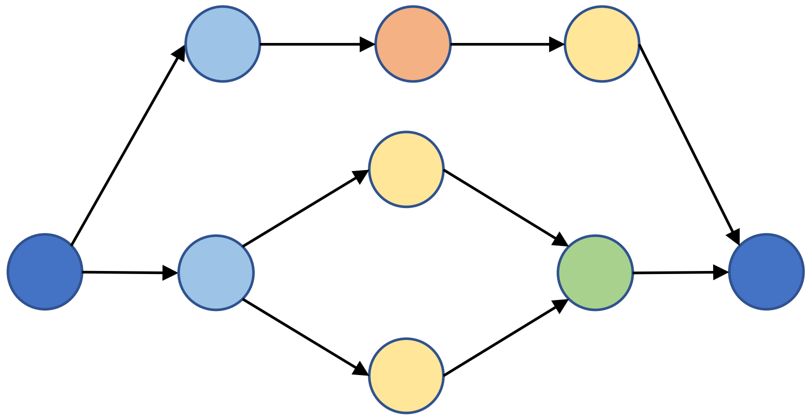


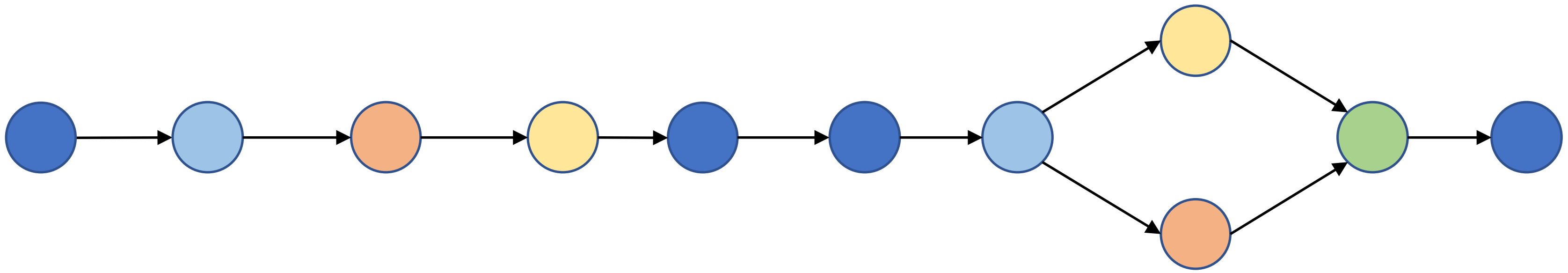


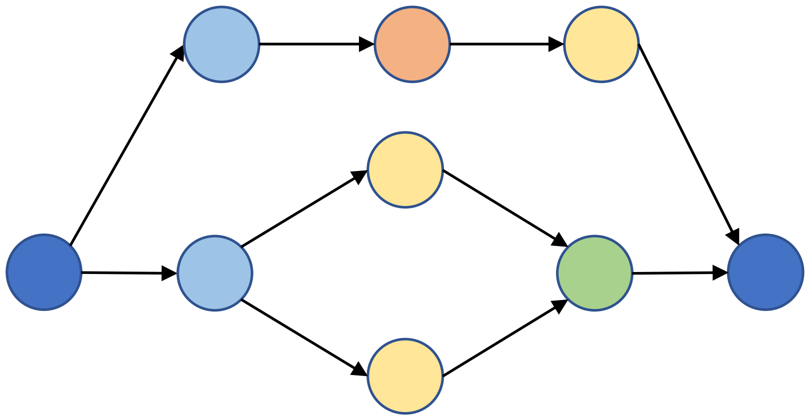


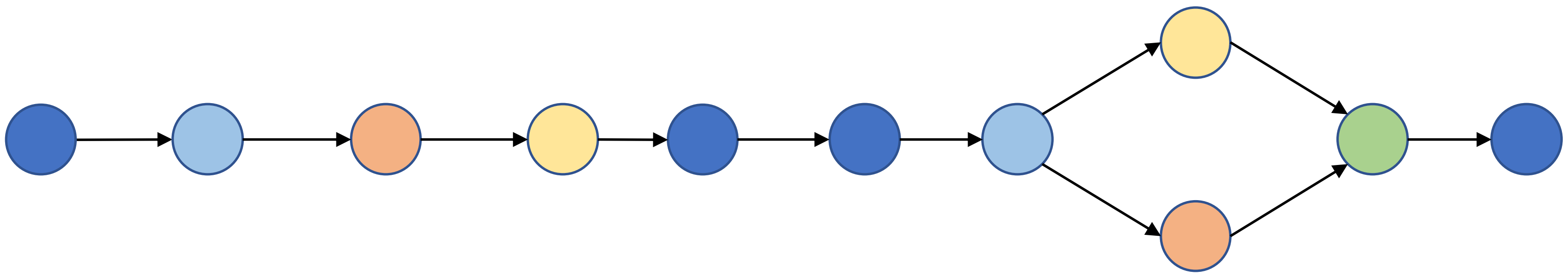


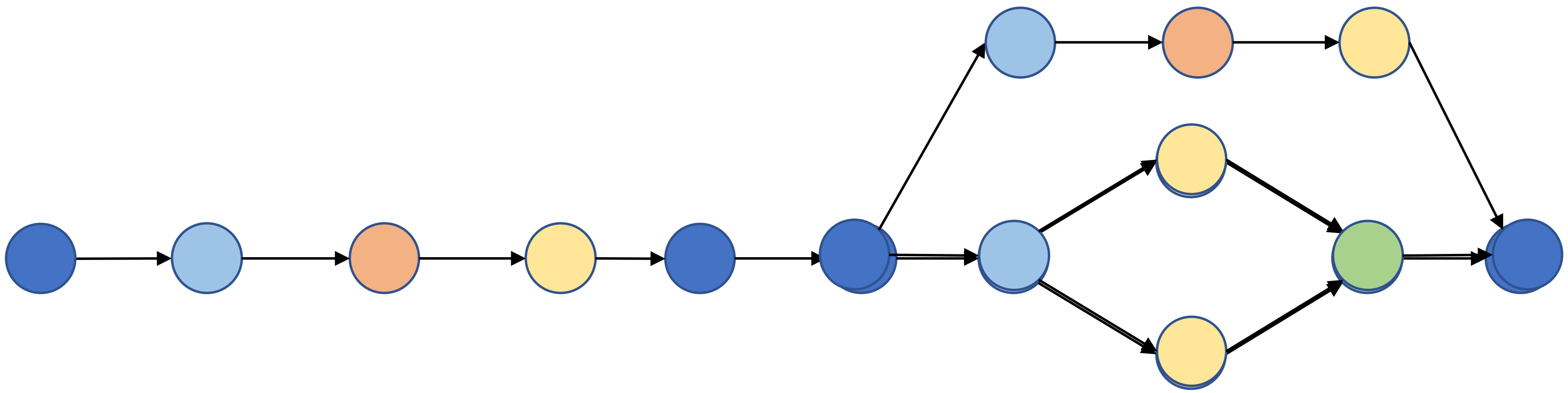


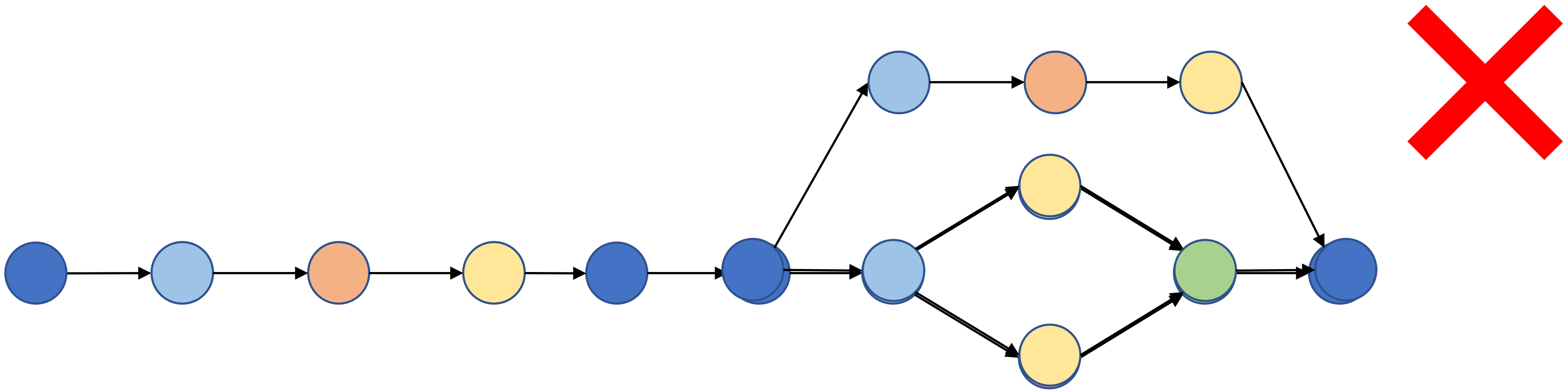


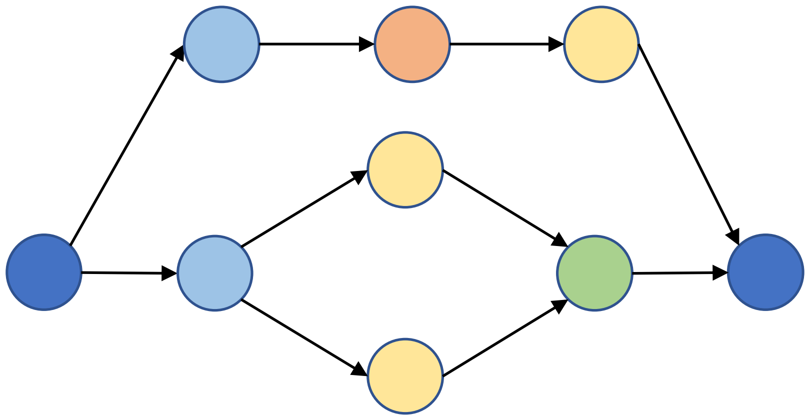


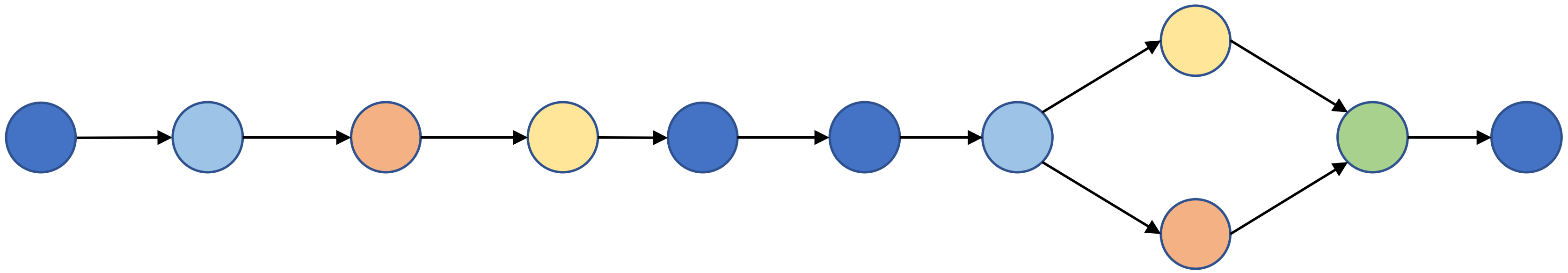




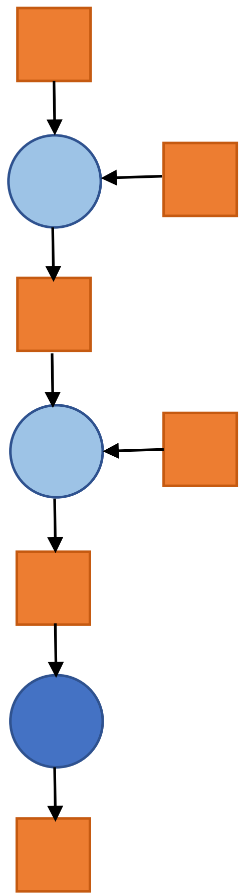








# *Elevating* a JIT graph to a PyTorch graph



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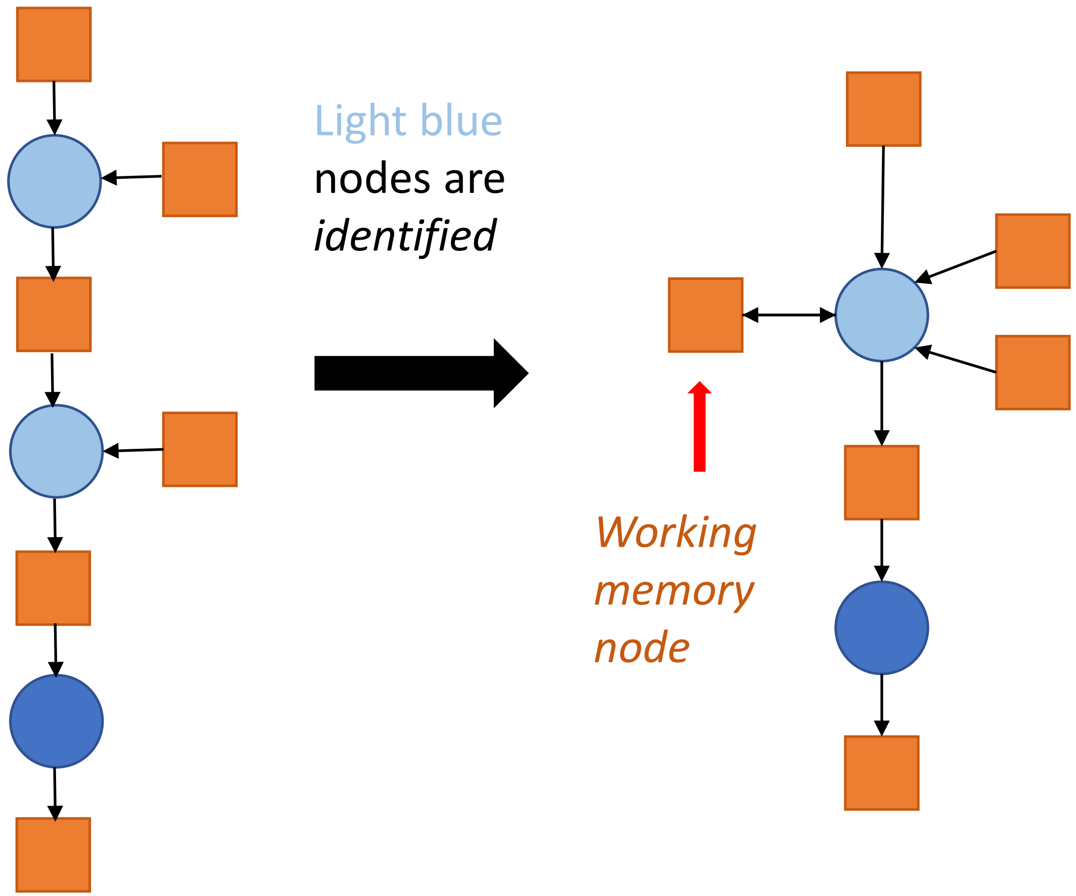

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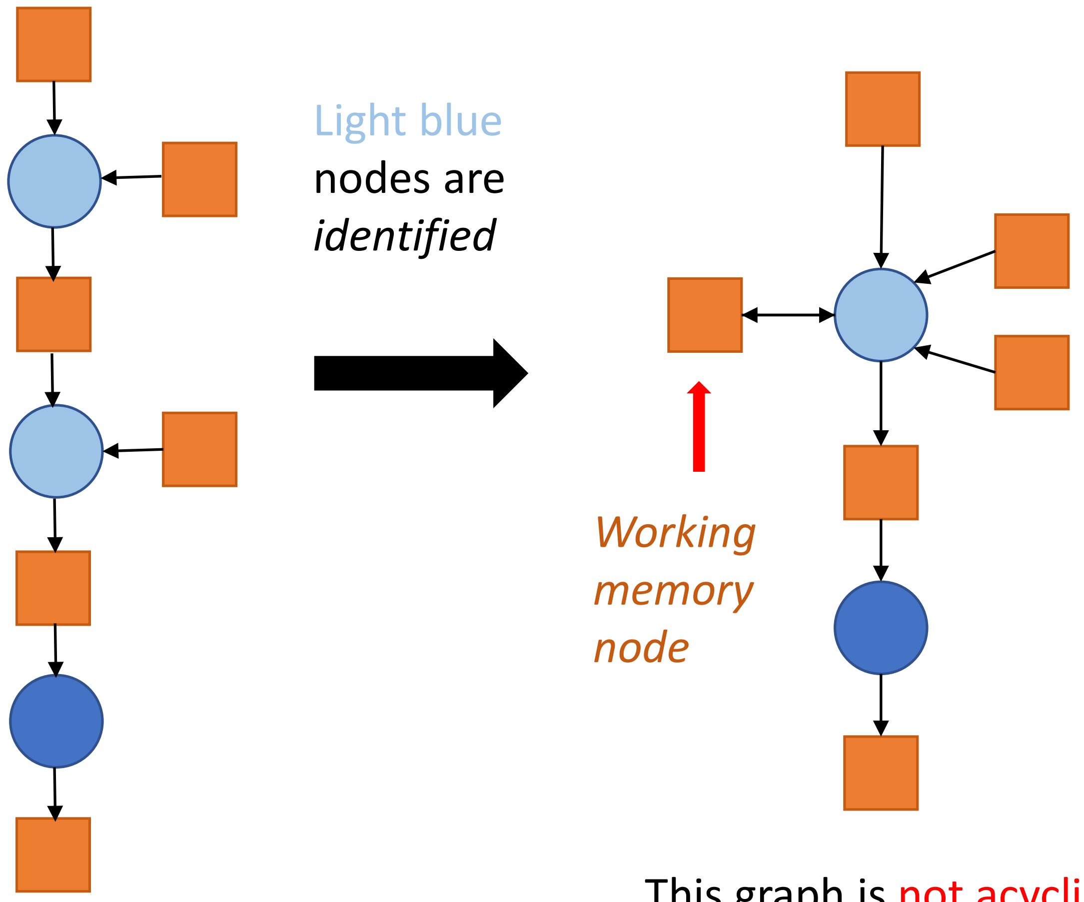


This graph is not acyclic!

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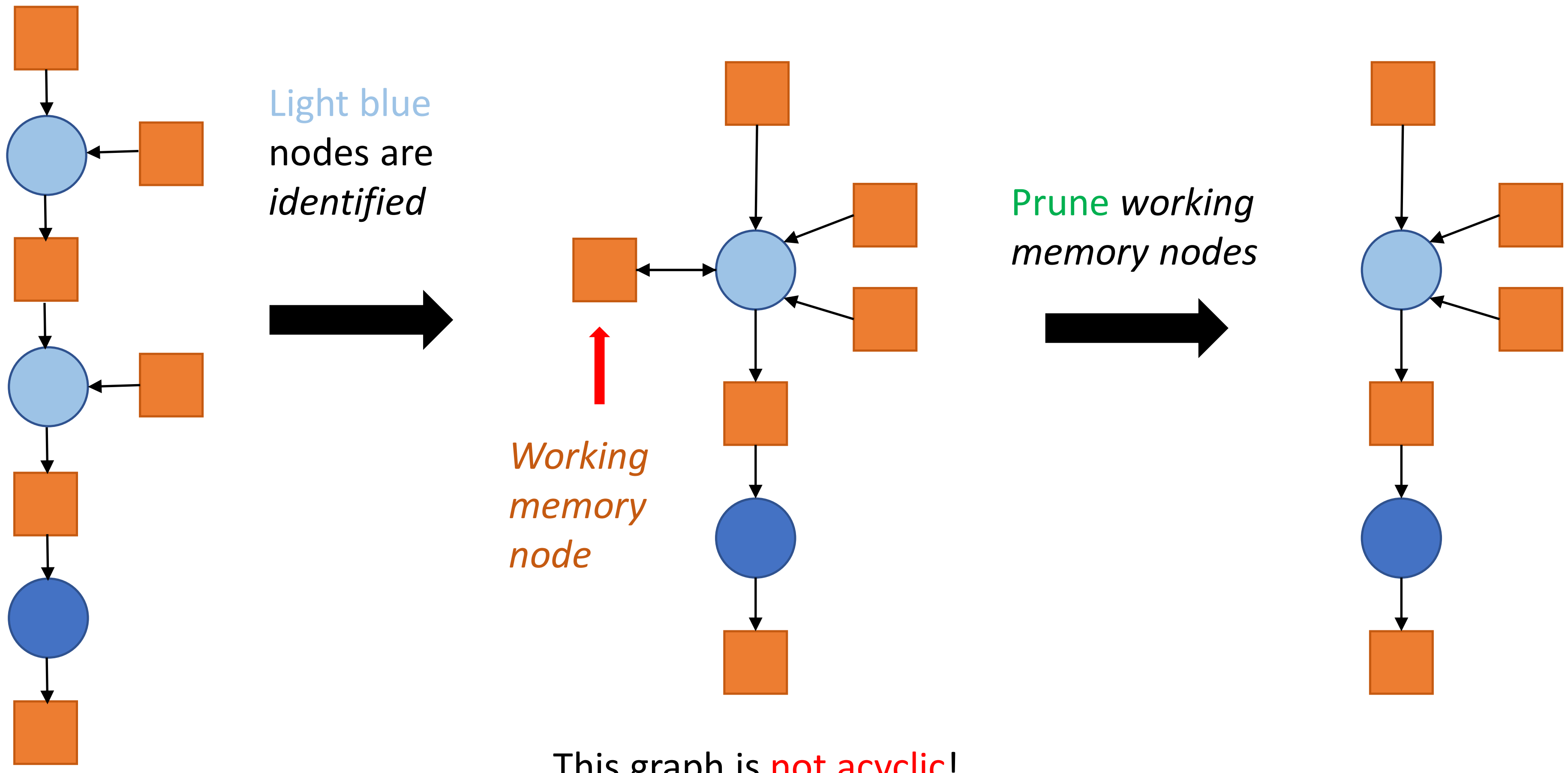


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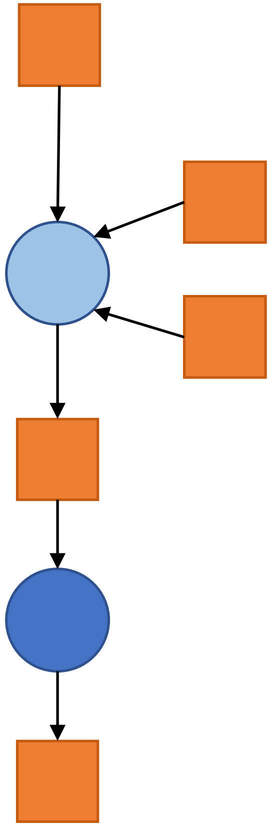
# Projecting a computational graph



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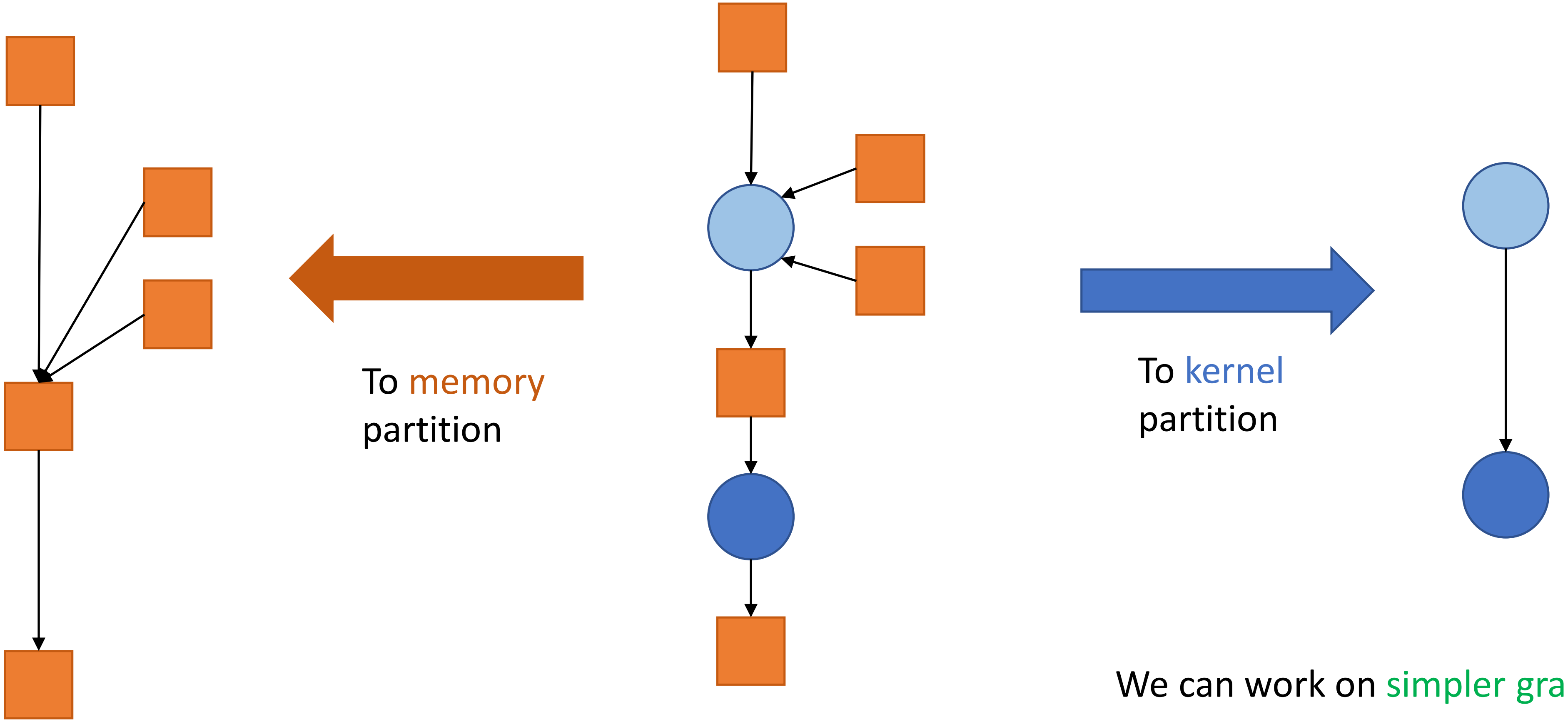


We can work on simpler graphs!

# Some last notes

- QuantLab and `quantlib` are released under the Apache 2.0 License
- This is a beta release: your feedback is our goal!
- Address communications to spmatteo@iis.ee.ethz.ch

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Special thanks…

… for assisting with the development and proofreading the notebooks:

Georg Rutishauser, Moritz Scherer

… for helping with the licensing and publication process:

Manuel Eggimann, Frank Kagan Gürkaynak

We hope to see you at the next edition!