

The *AMARETTO framework: a regulatory network inference tool for multi-omics & imaging data fusion across systems and diseases

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Demo: Mohsen Nabian, Ph.D. (mnabian@broadinstitute.org)

Harvard Medical School, Brigham and Women's Hospital, Broad Institute of MIT and Harvard

Big Data in Biomedicine: Big Data Modeling in Human Diseases

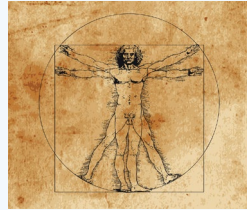
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Multi-Omics & Imaging Data Fusion across Systems and Diseases

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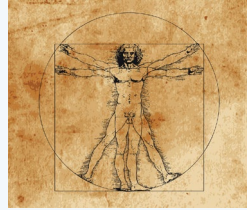
Patient Studies



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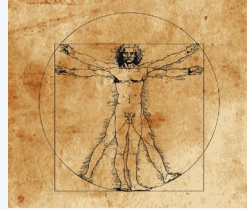
Decipher disease heterogeneity

Multi-omics: (epi)genetics & functional genomics
Driver discovery via regulatory network inference

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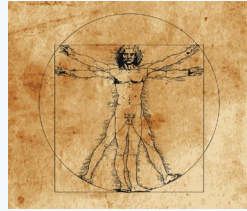
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Bulk & single-cell multi-omics
Non-invasive & histopathology imaging

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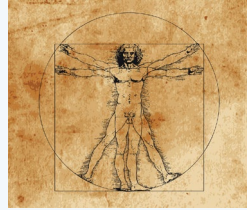
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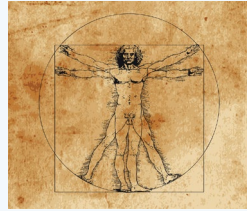
Perturbation studies

Genetic perturbations for driver discovery
Chemical perturbations for drug discovery

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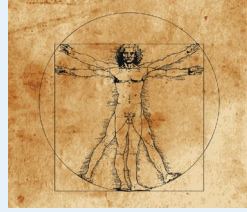
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Multi-omics & imaging
Genetic & chemical perturbations

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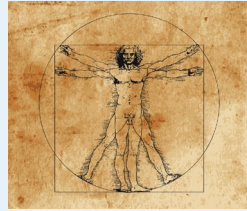
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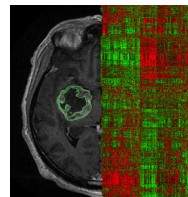
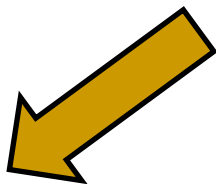
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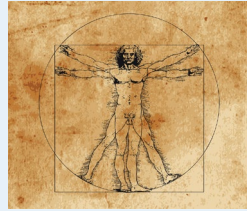


Disease (sub)typing

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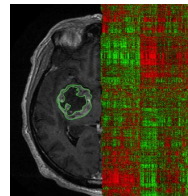
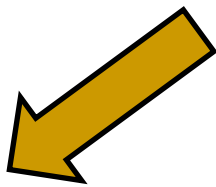
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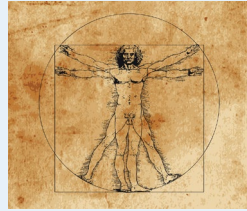


Driver discovery

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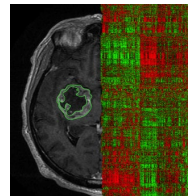
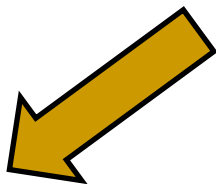
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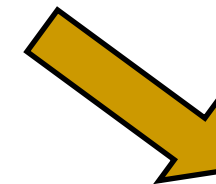
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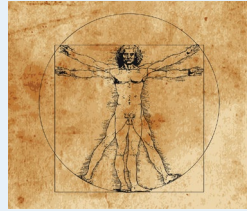


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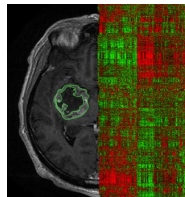
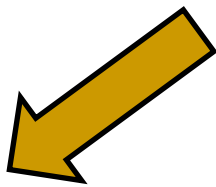
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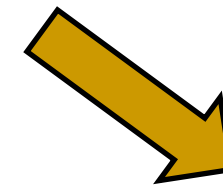
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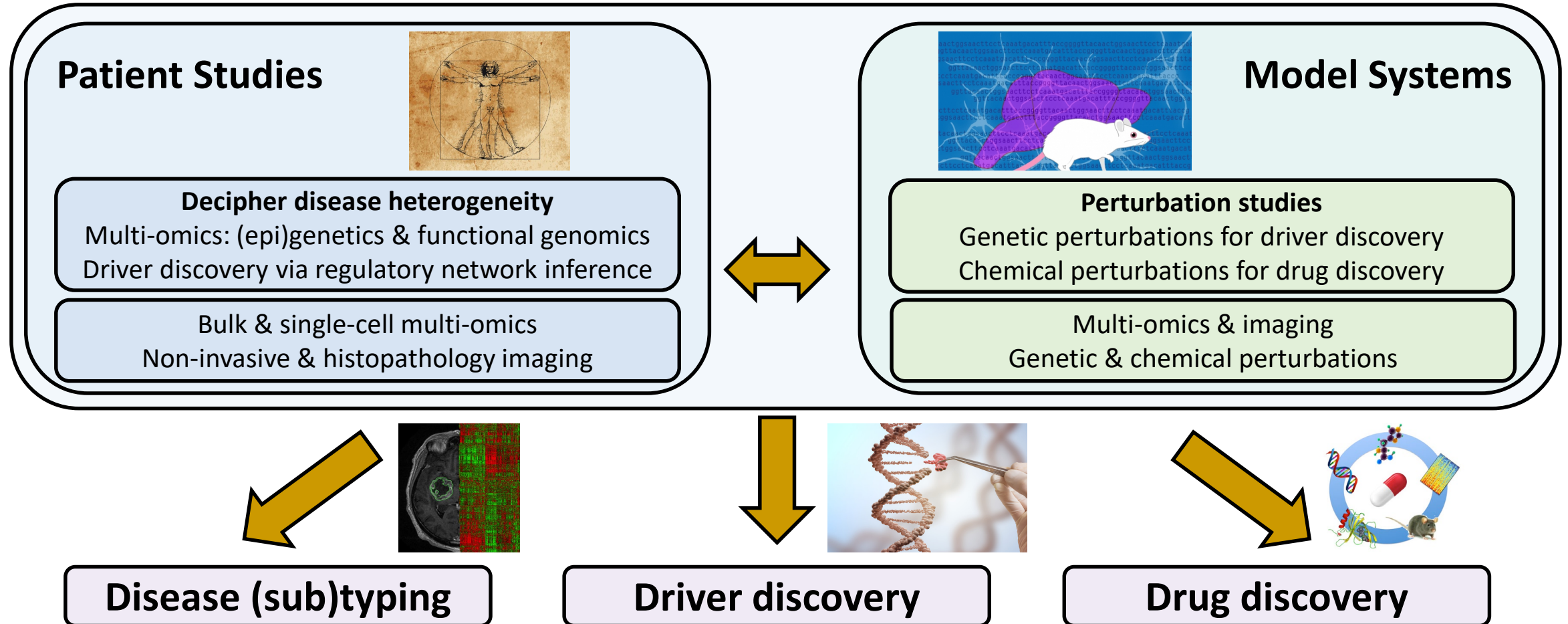


Drug discovery

Large publicly available archives provide us with complementary views of human disease.

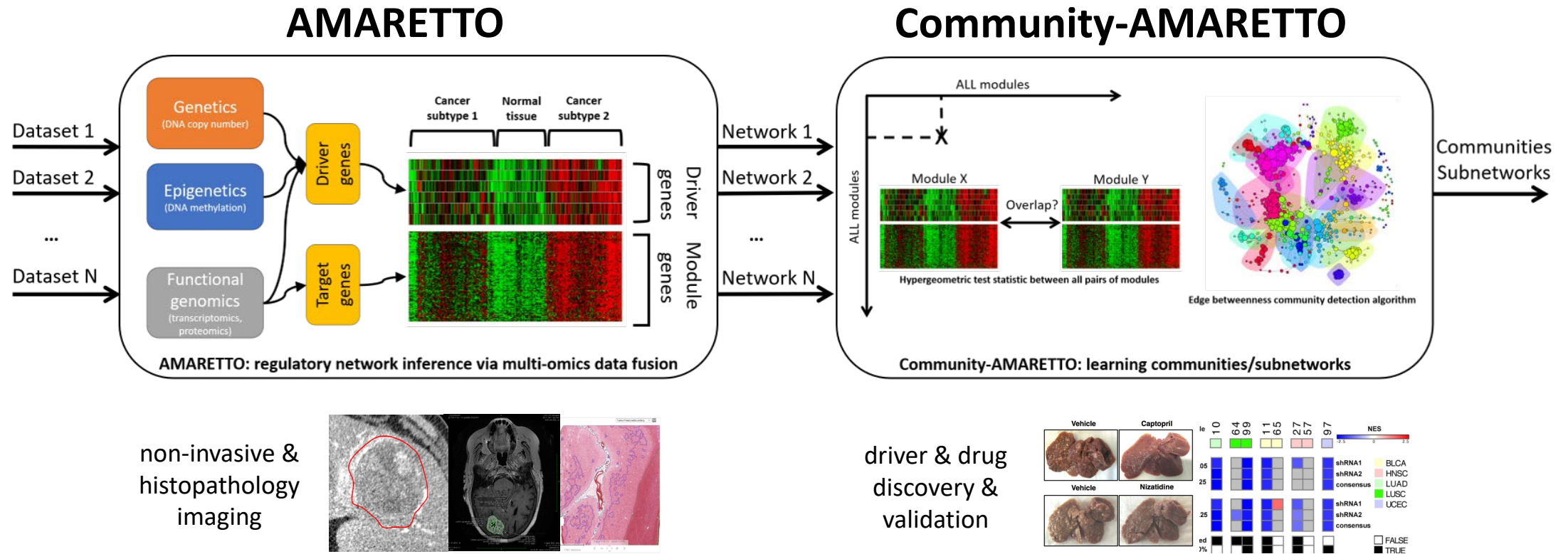
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Can we learn more powerful models by translating knowledge across different domains?

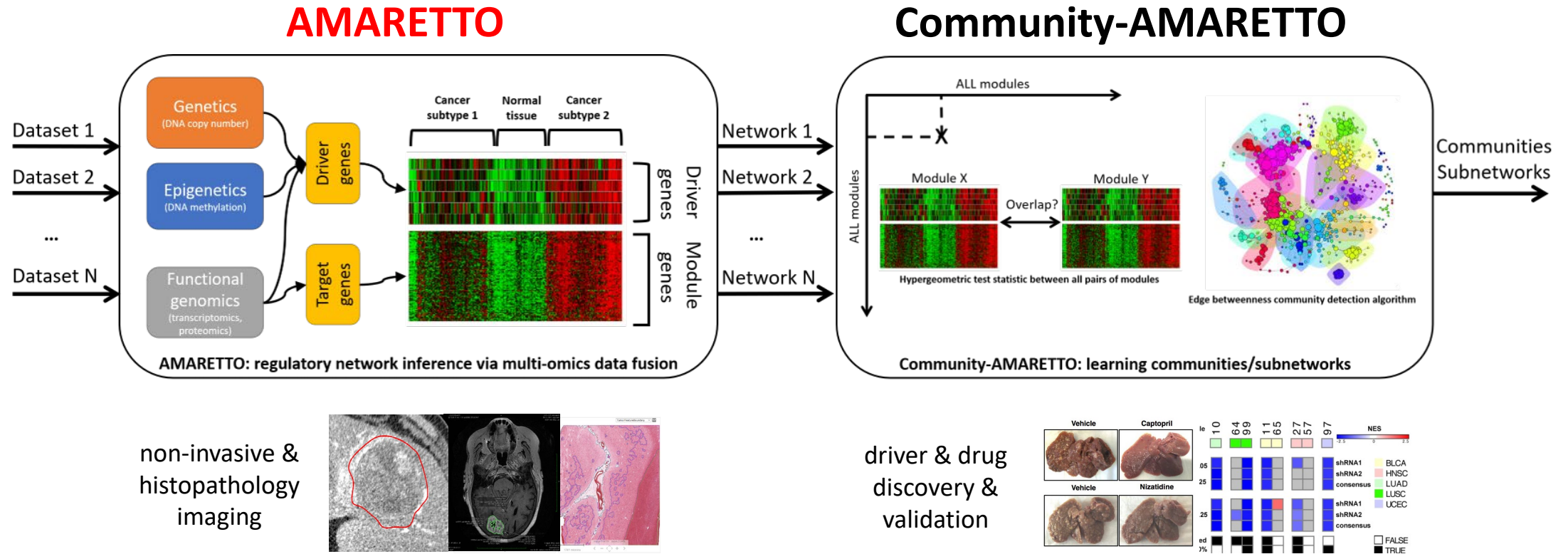
The *AMARETTO framework



The *AMARETTO framework:

1. the **AMARETTO** algorithm for inferring regulatory networks via multi-omics and imaging data fusion
2. the **Community-AMARETTO** algorithm for learning subnetworks shared/distinct across systems and diseases

The *AMARETTO framework



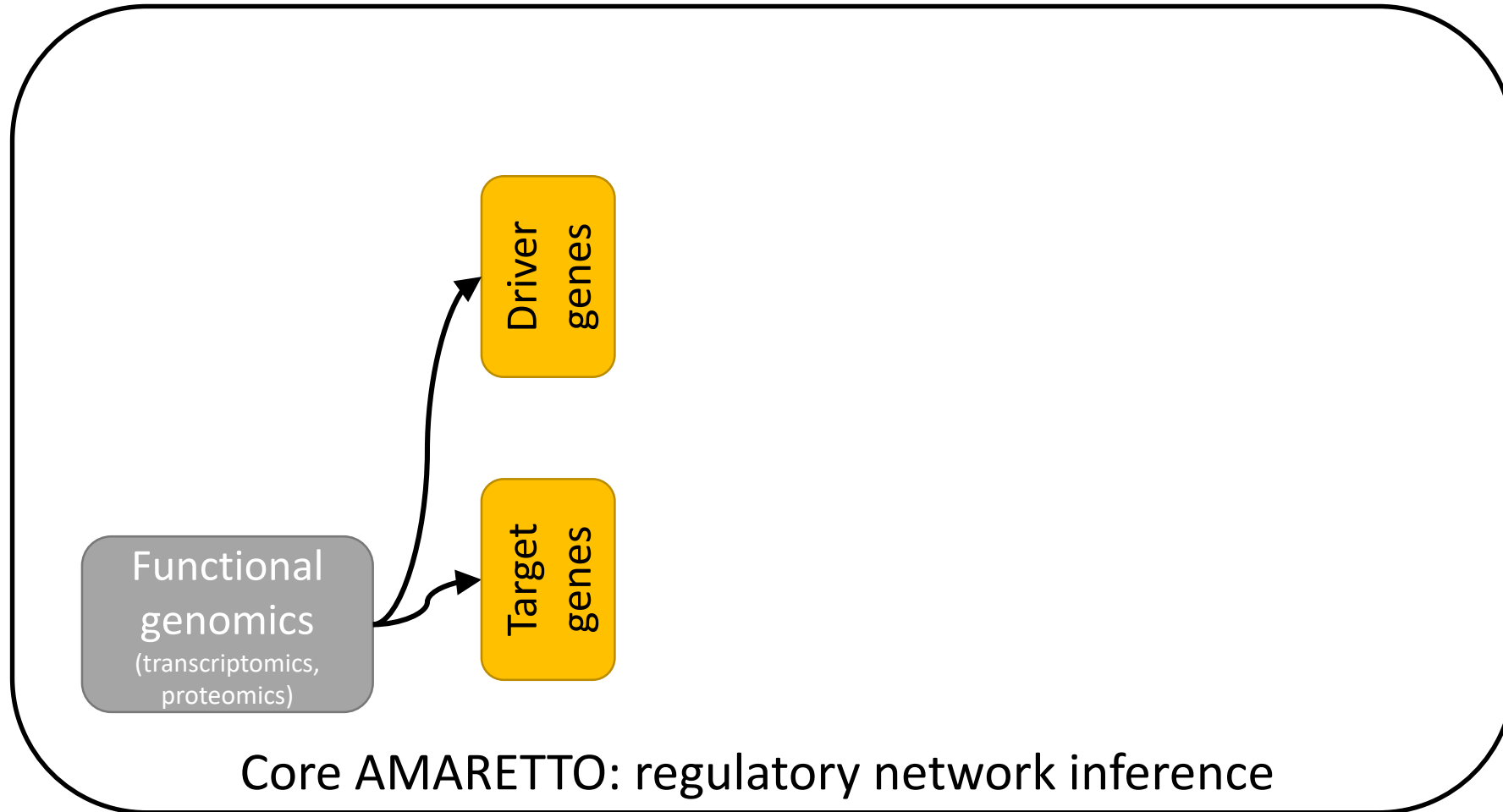
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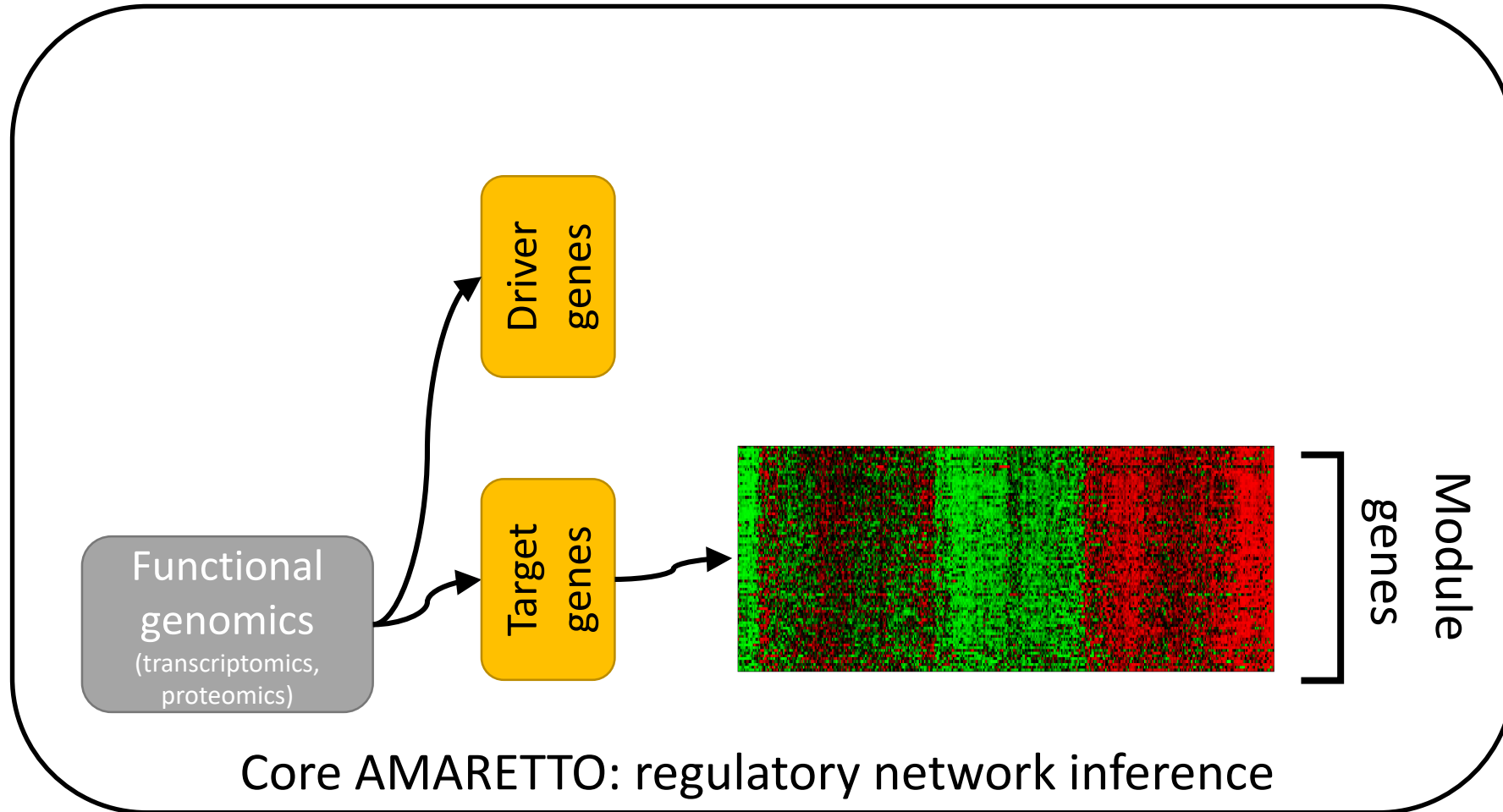
AMARETTO for regulatory network inference within systems and diseases



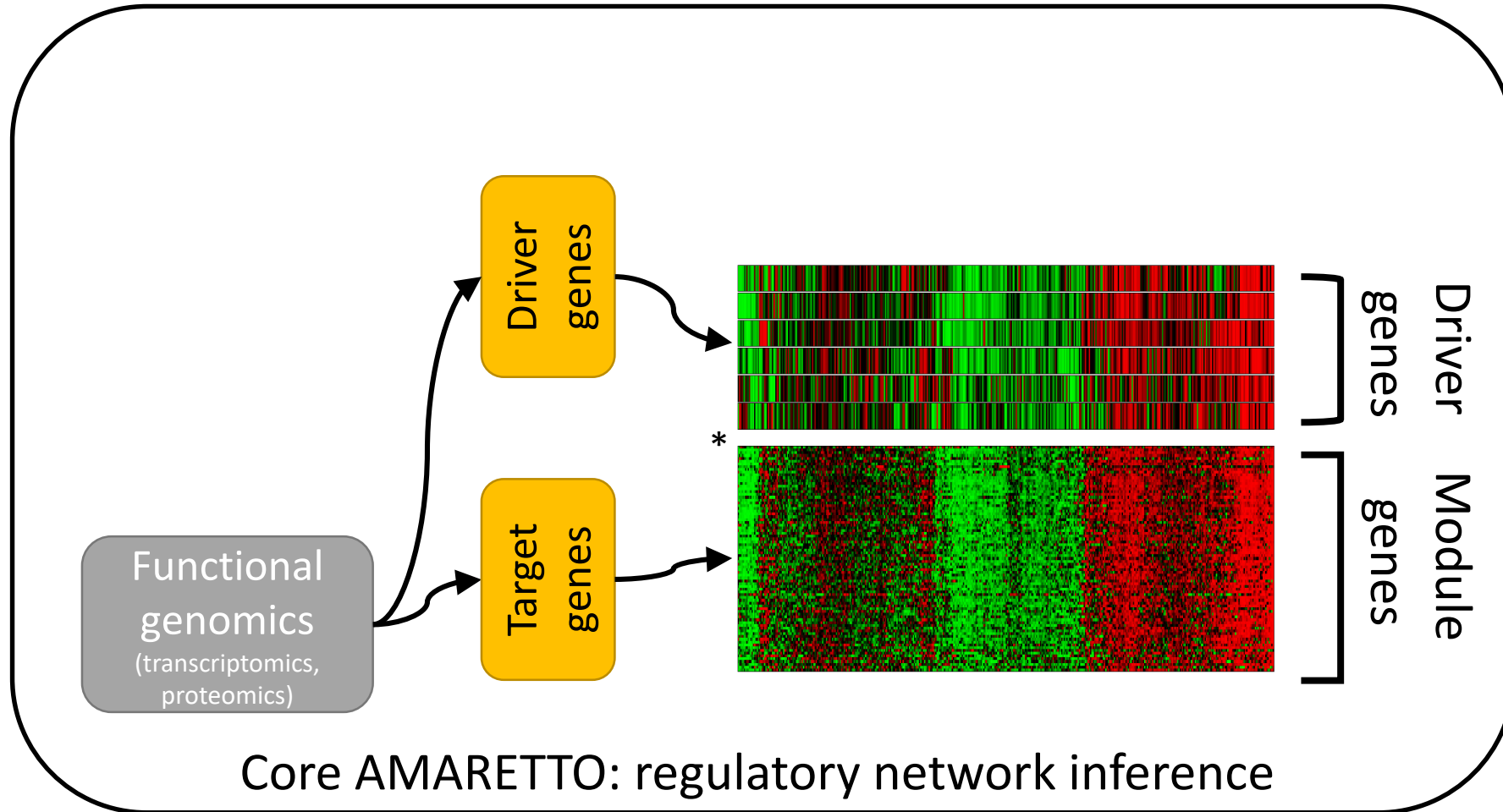
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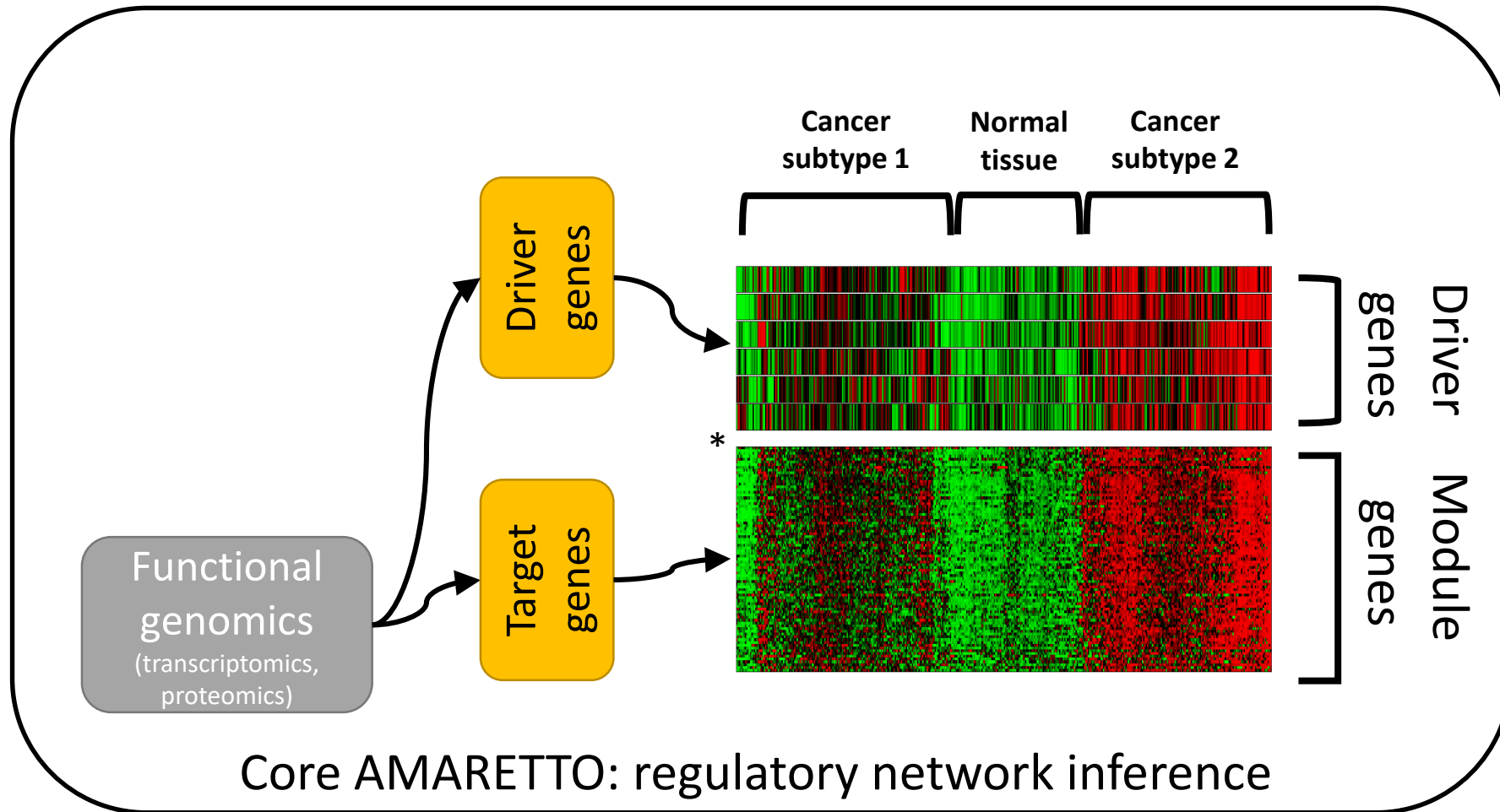


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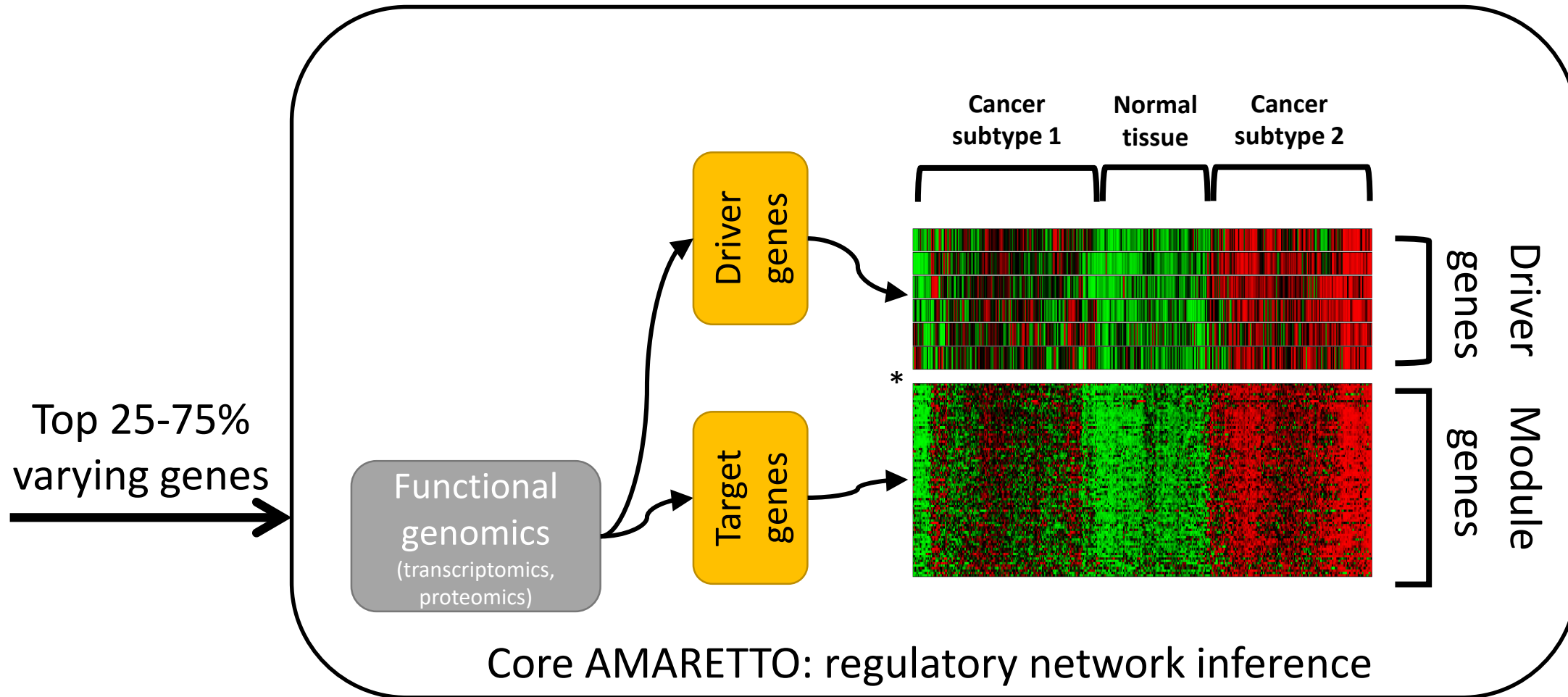
(*) Regularized regression: Lee *et al.*, PLoS Genetics 2009; Zou and Hastie, J R Stat Soc 2005; Tibshirani, J R Stat Soc 1996

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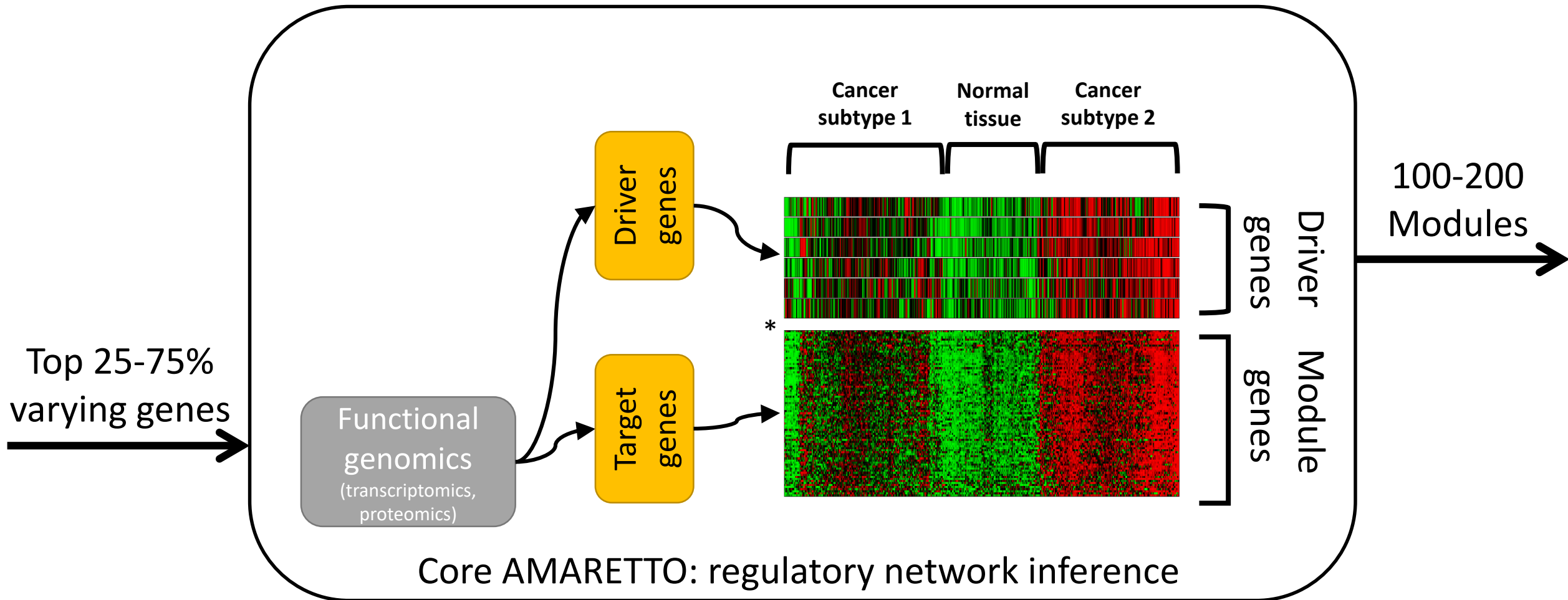
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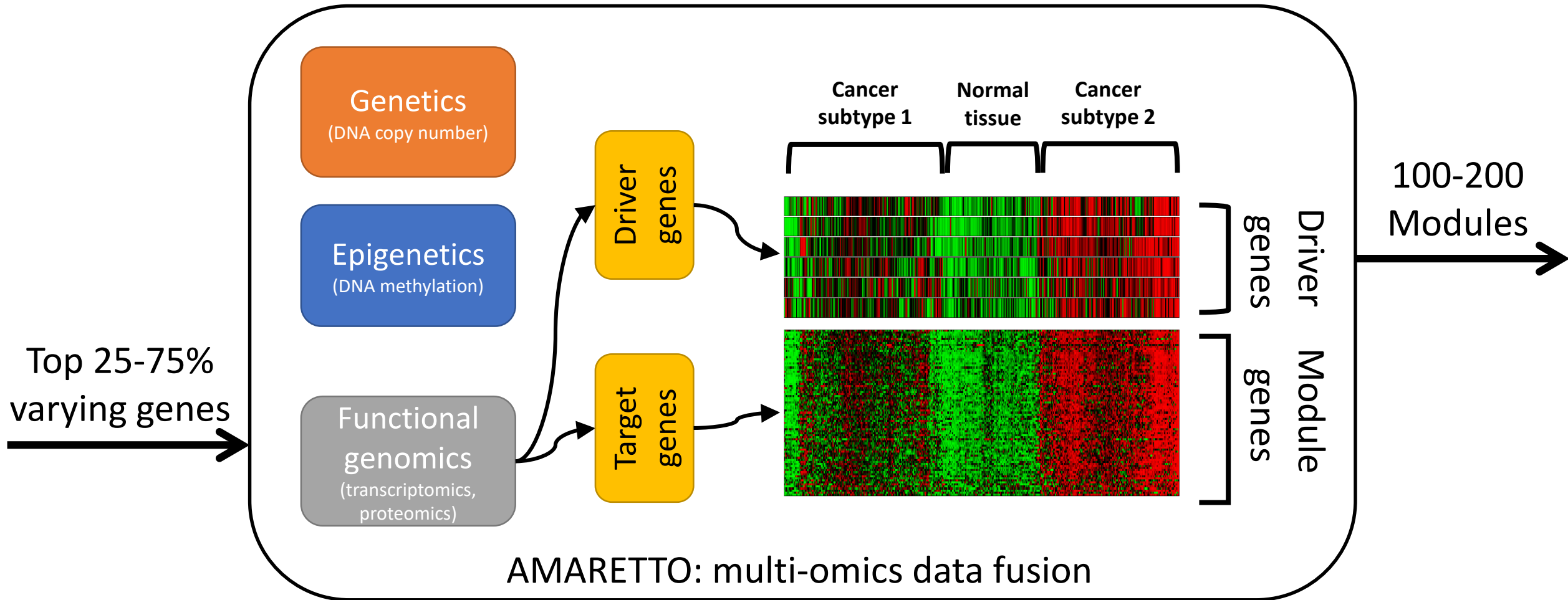
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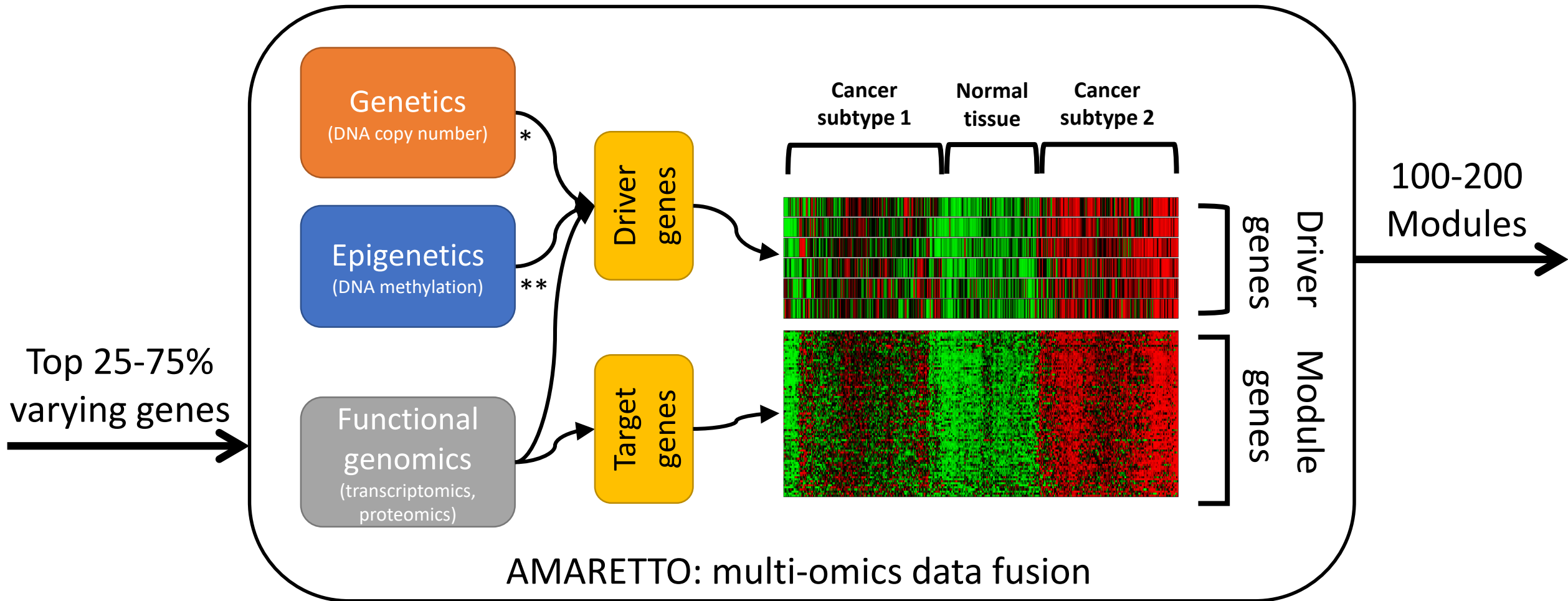


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AMARETTO for multi-omics data fusion within systems and diseases



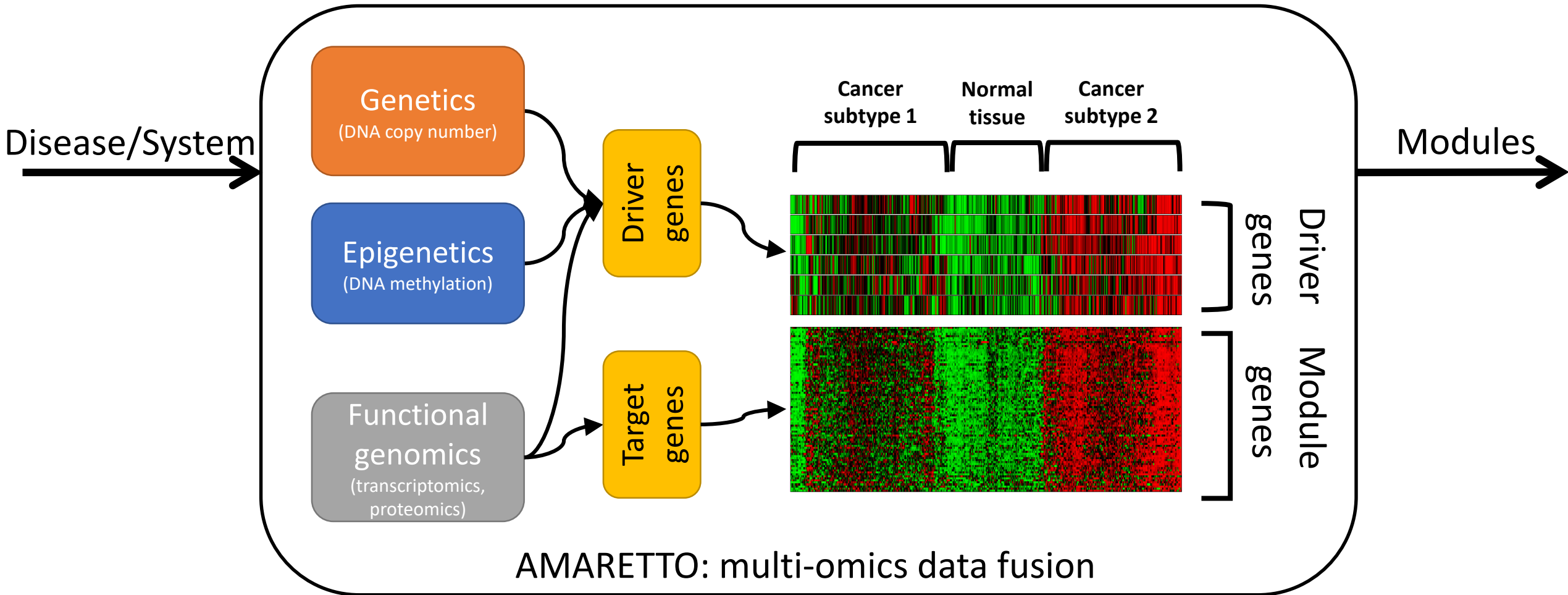
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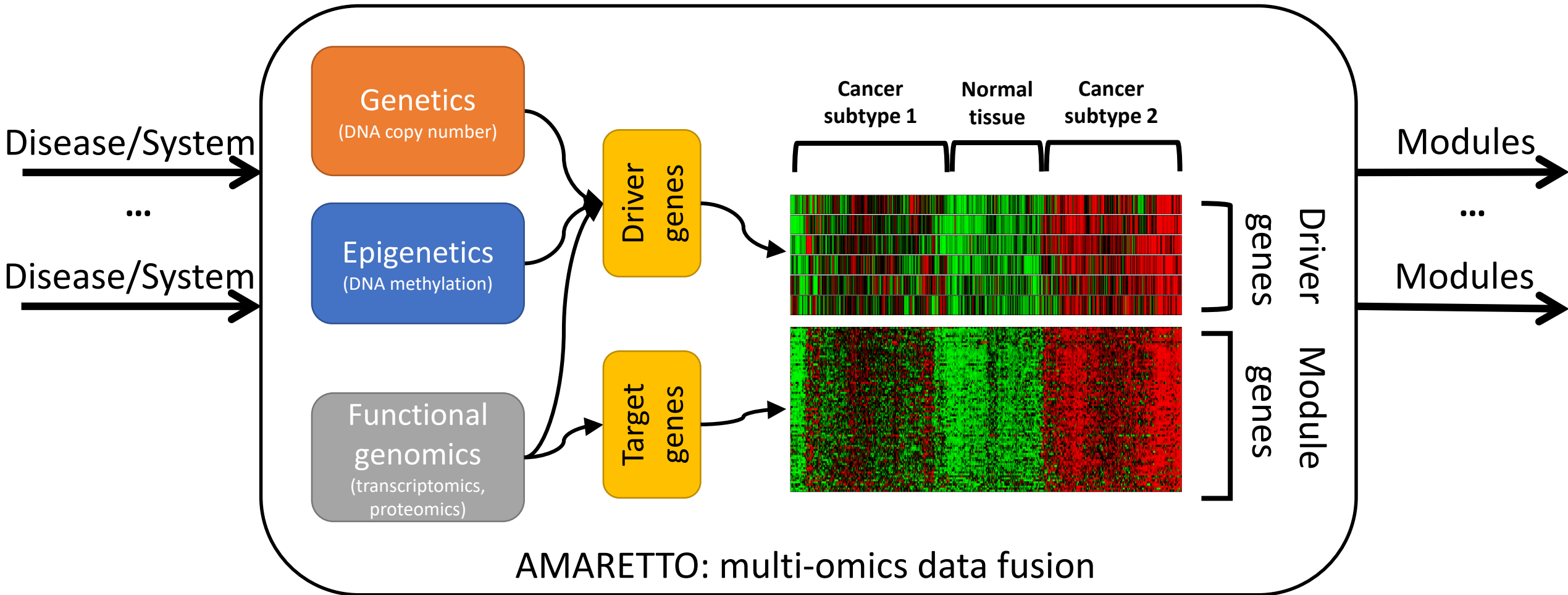
(*) GISTIC: Mermel *et al.*, Genome Biology 2011; Beroukhim *et al.*, Nature 2010

(**) MethylMix: Gevaert, Bioinformatics 2015; Gevaert *et al.*, Genome Biology 2015; Cedoz *et al.*, Bioinformatics 2018

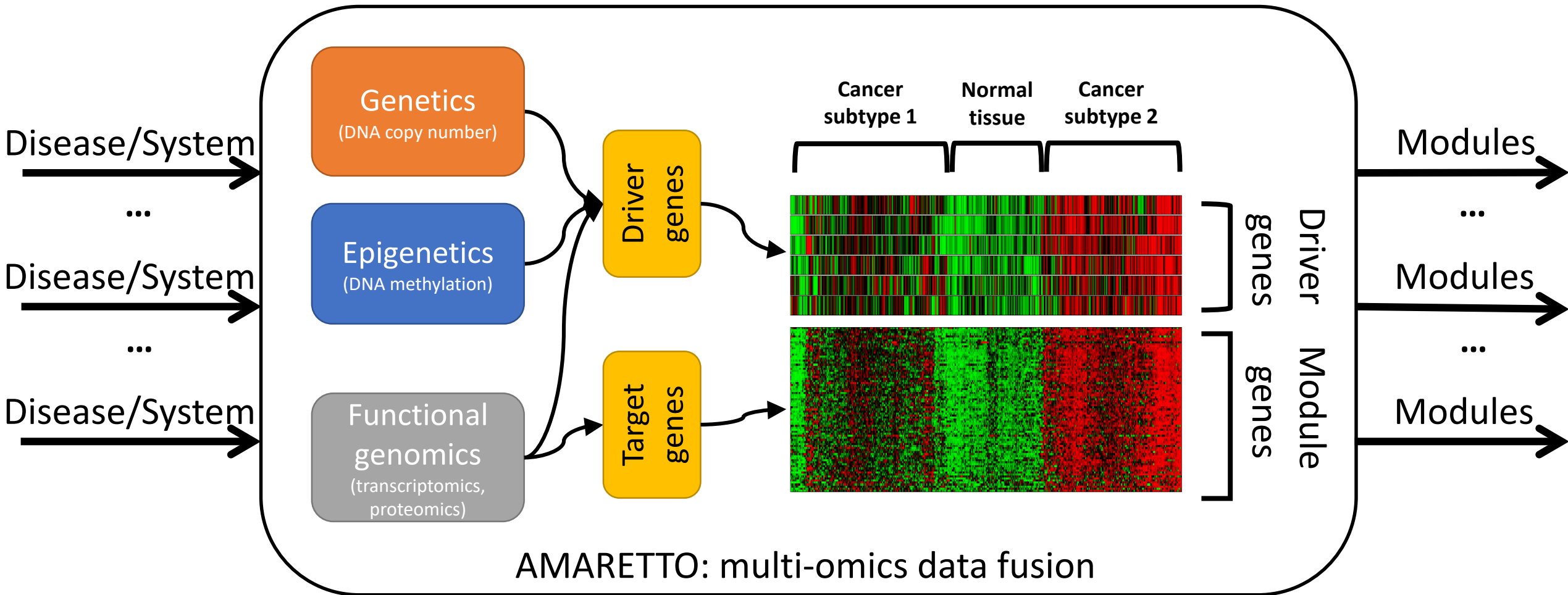
AMARETTO for multi-omics data fusion in multiple systems and diseases



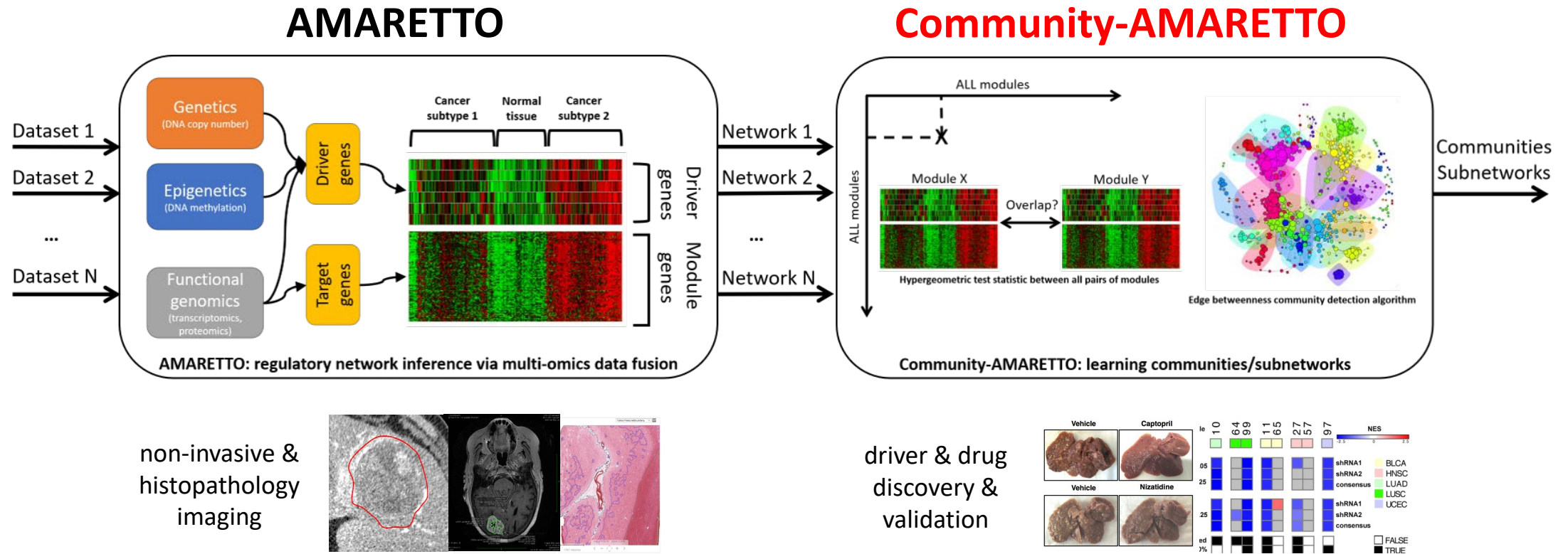
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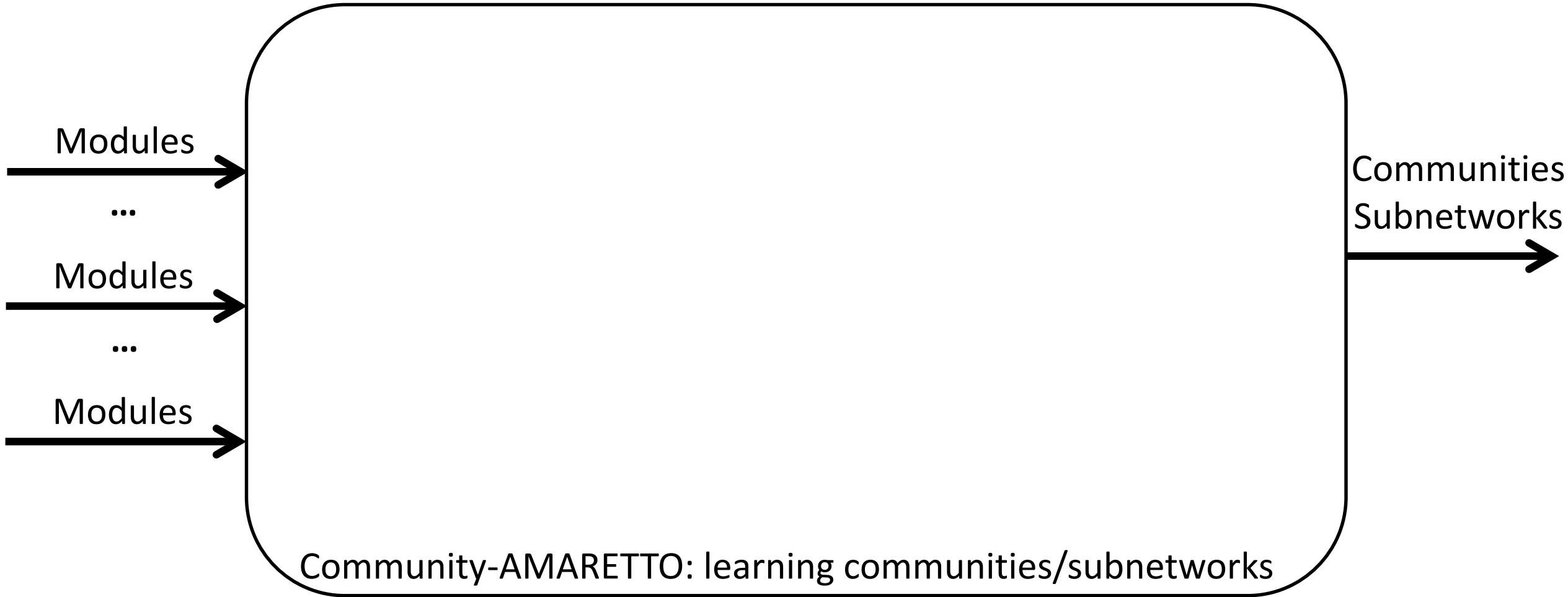
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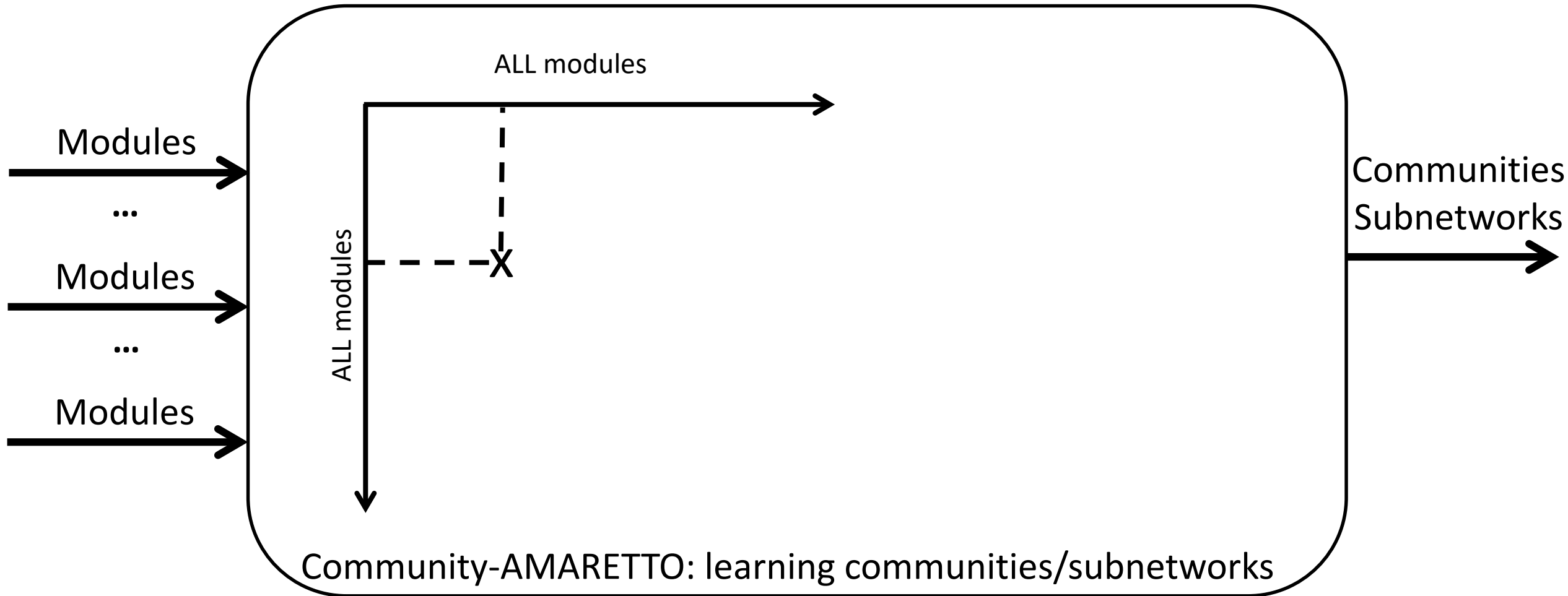
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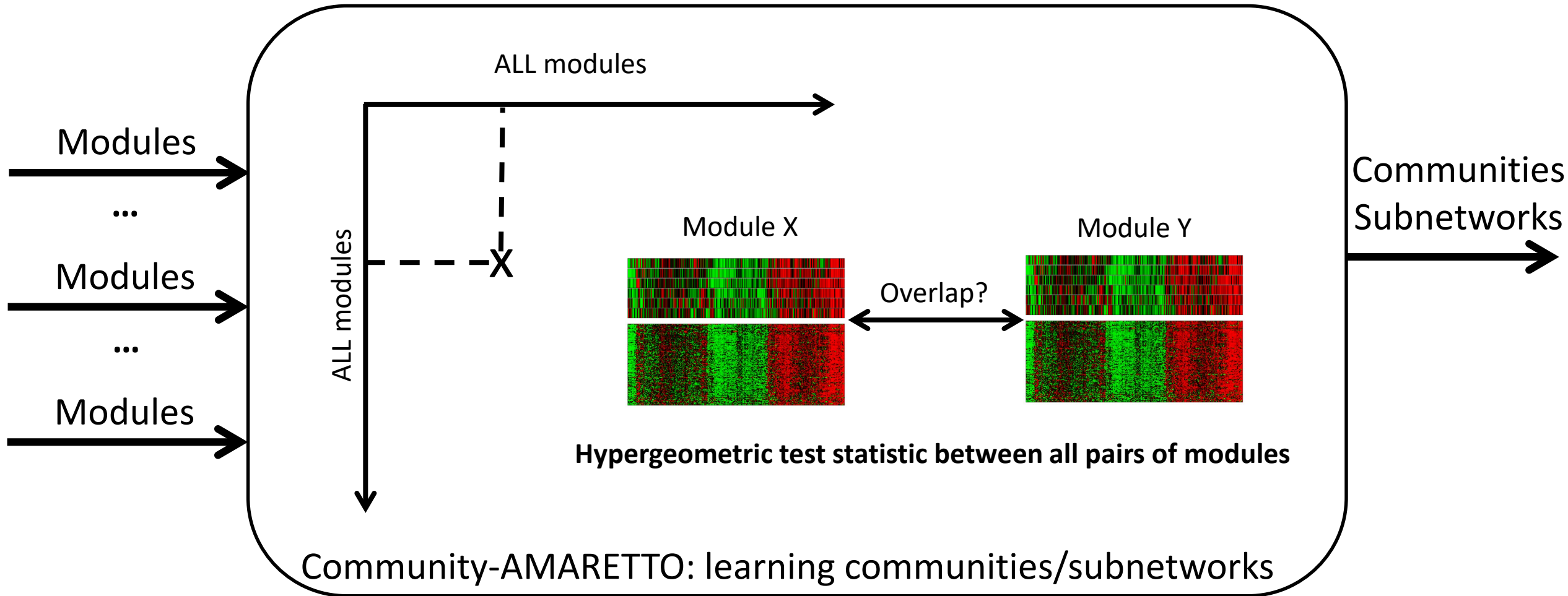
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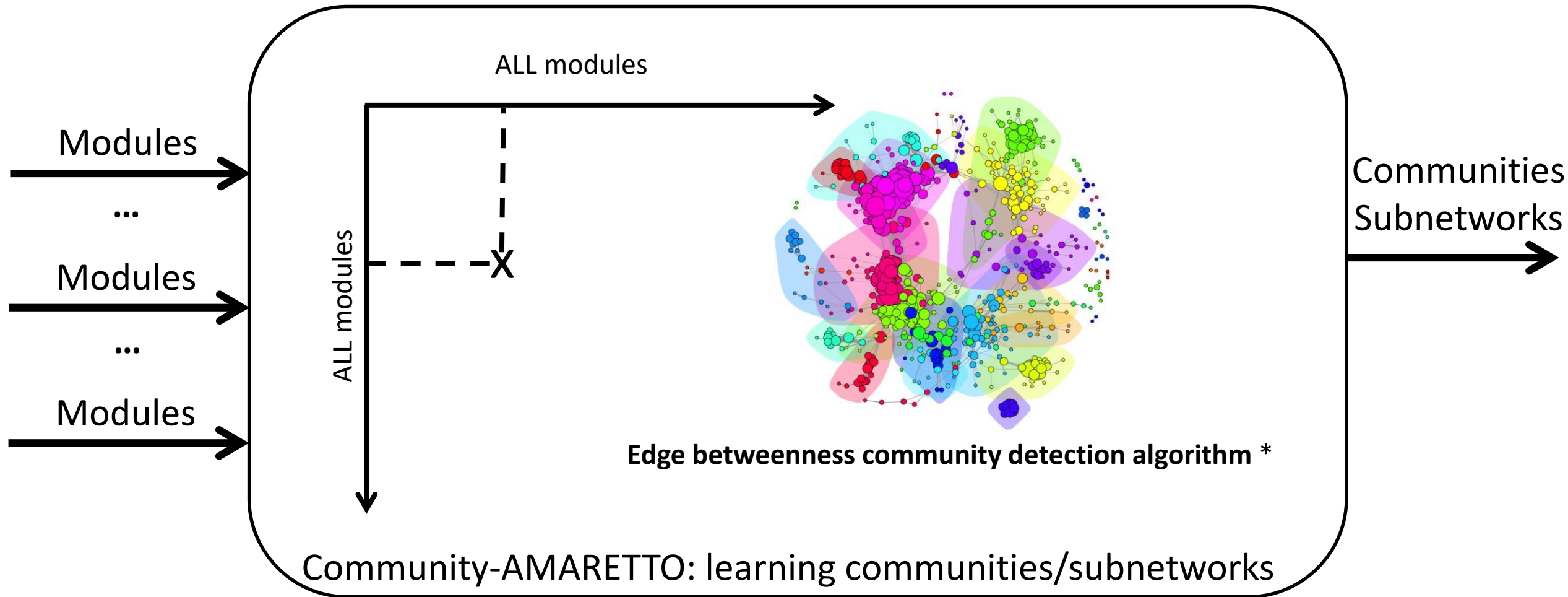
AMARETTO for learning subnetworks across systems and diseases



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(*) Girvan and Newman, Physical Review E. 2004

Functionalities for optimization and downstream analytics

Optimal generalization performance

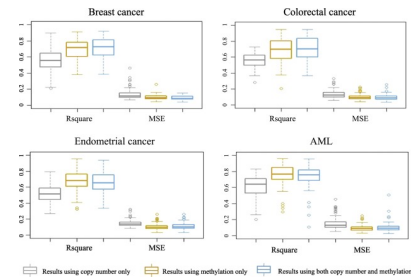
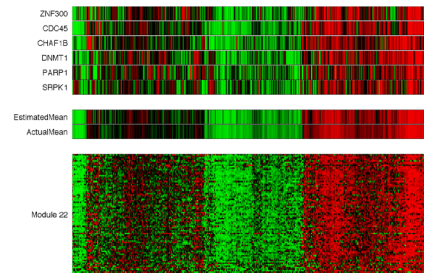
Stratification for disease phenotypes

Annotation of functional categories

Association with imaging features

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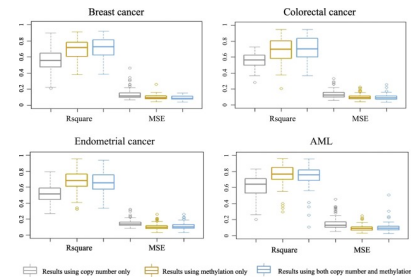
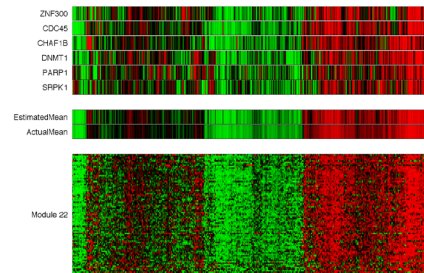
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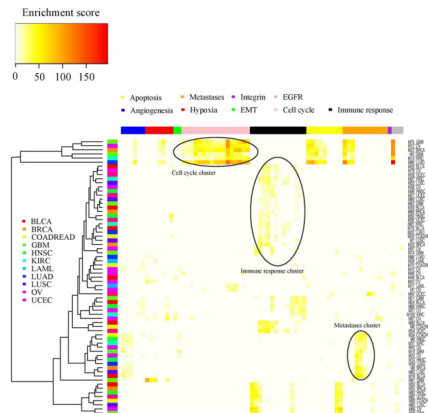
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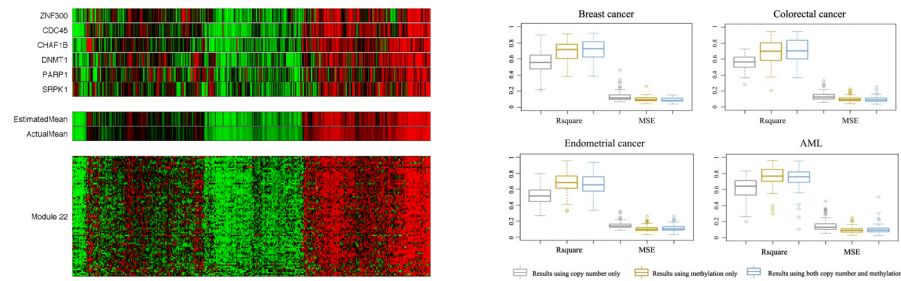
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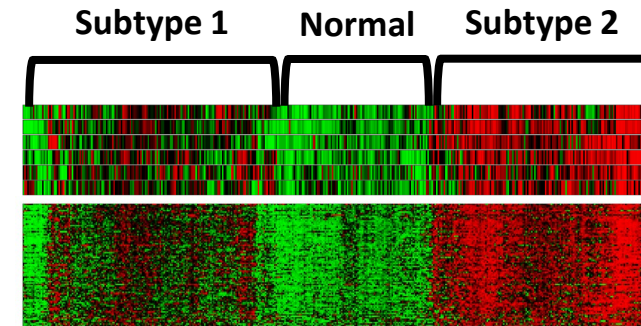
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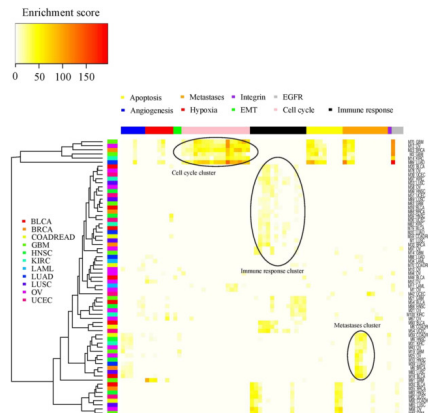
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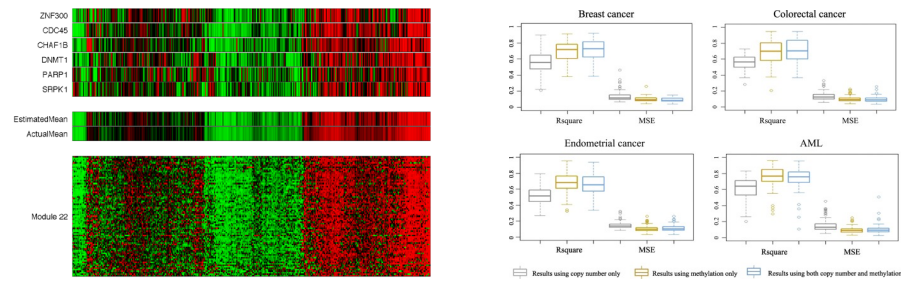
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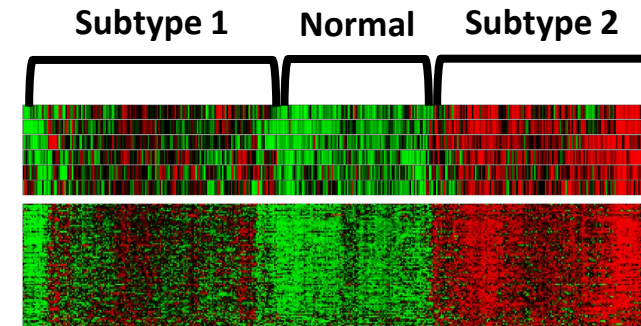
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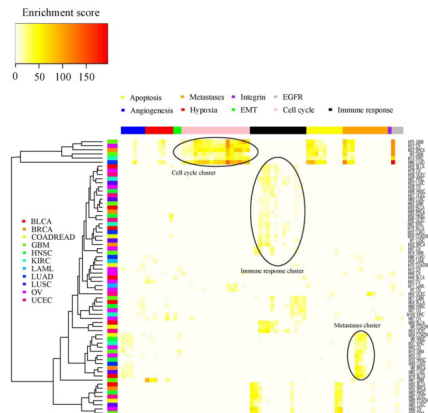
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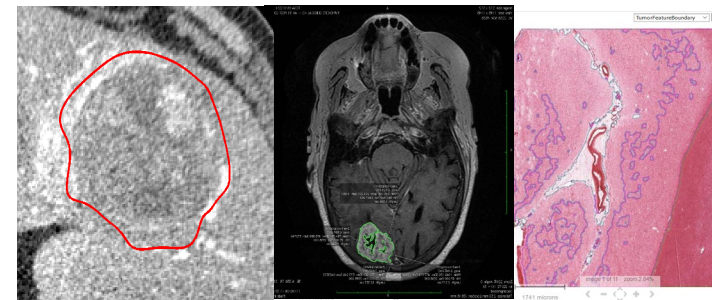
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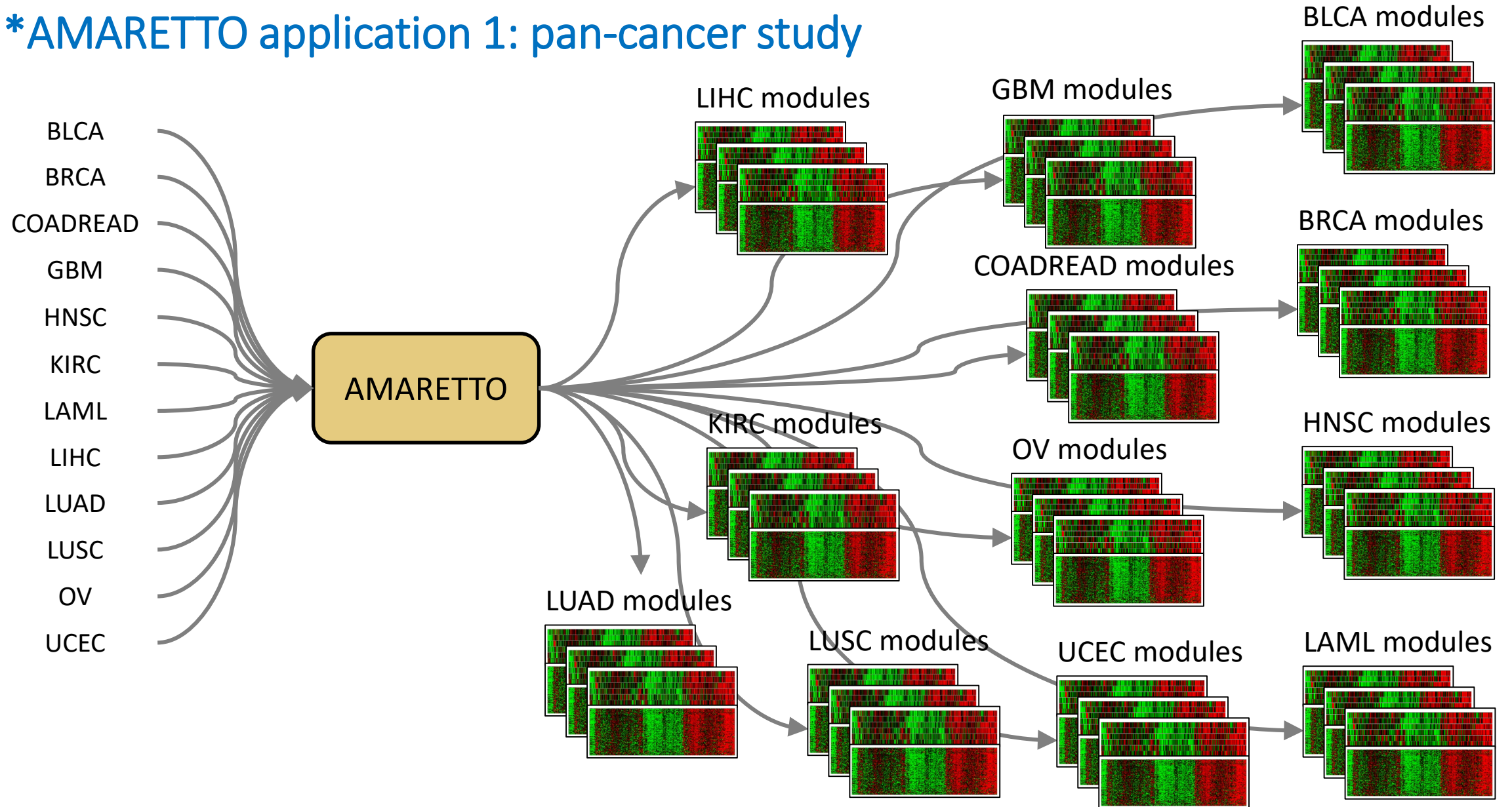
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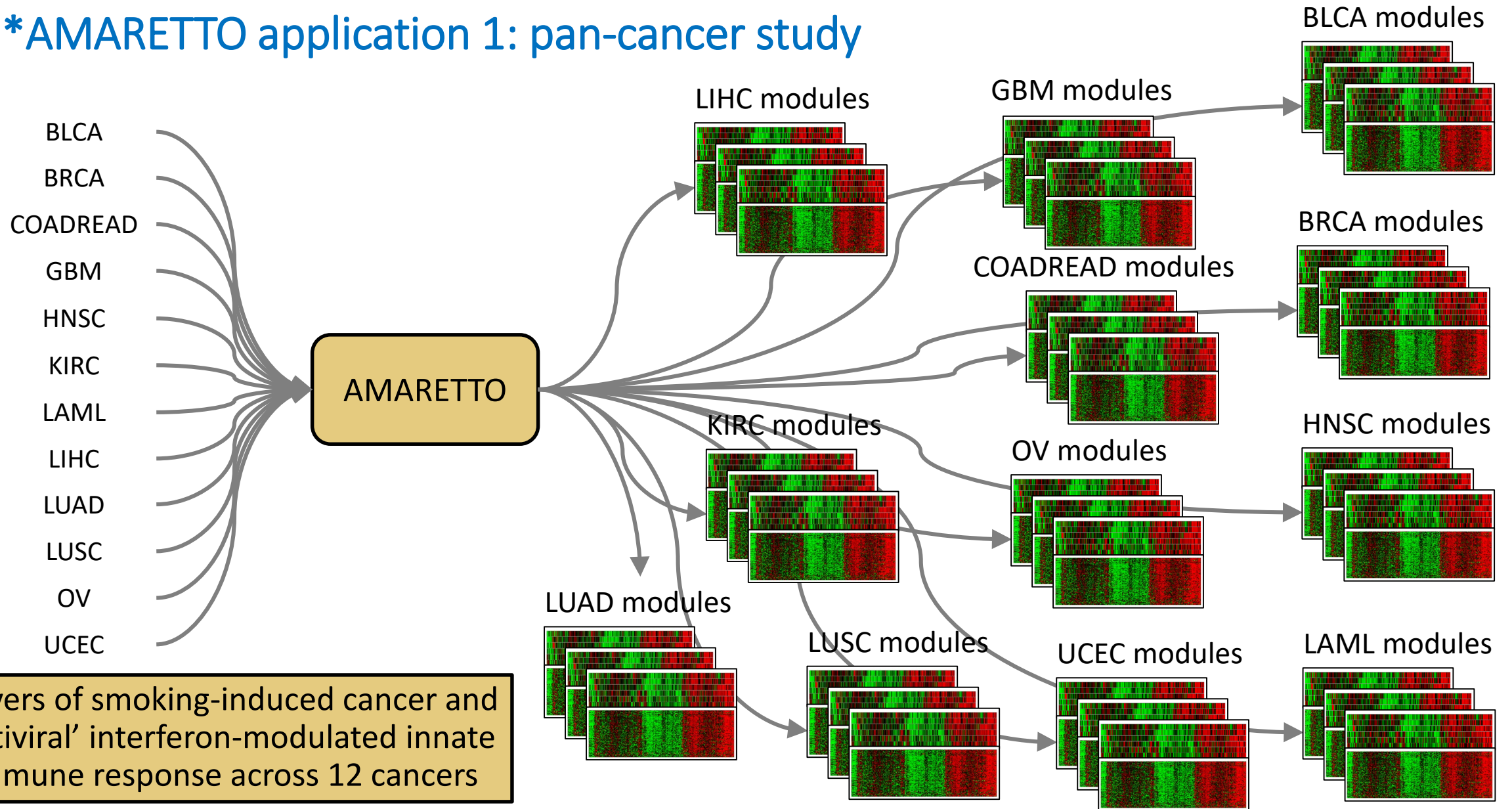
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*AMARETTO application 1: pan-cancer study

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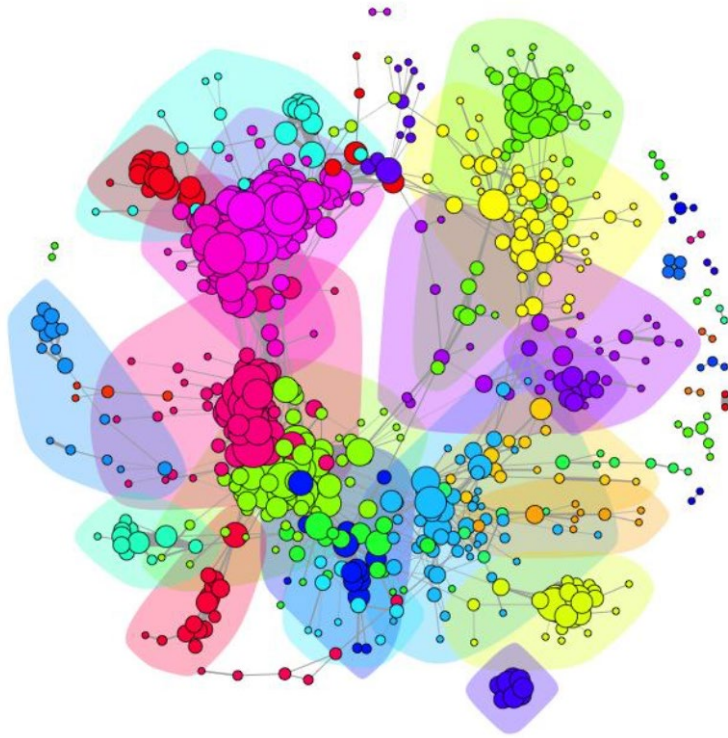


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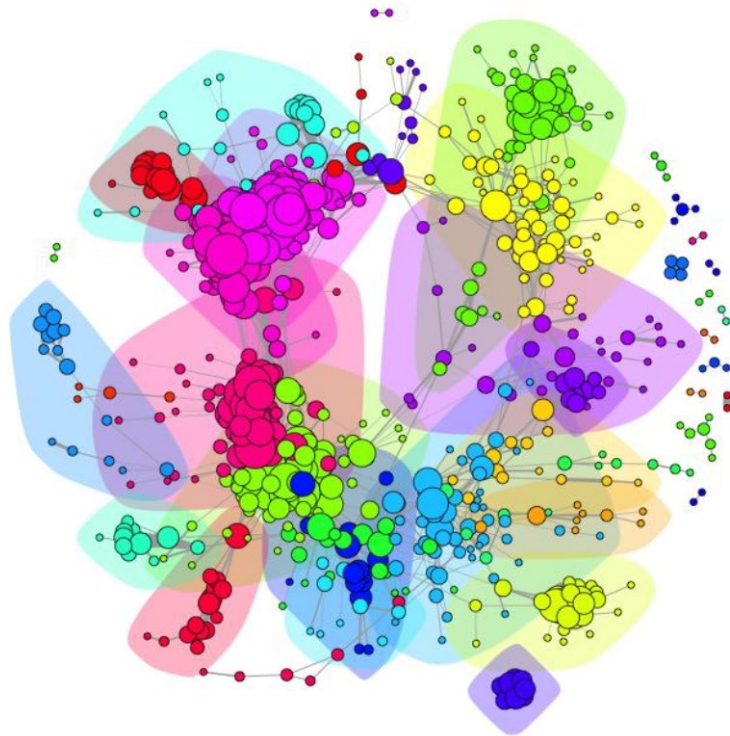
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Pan-cancer communities or subnetworks

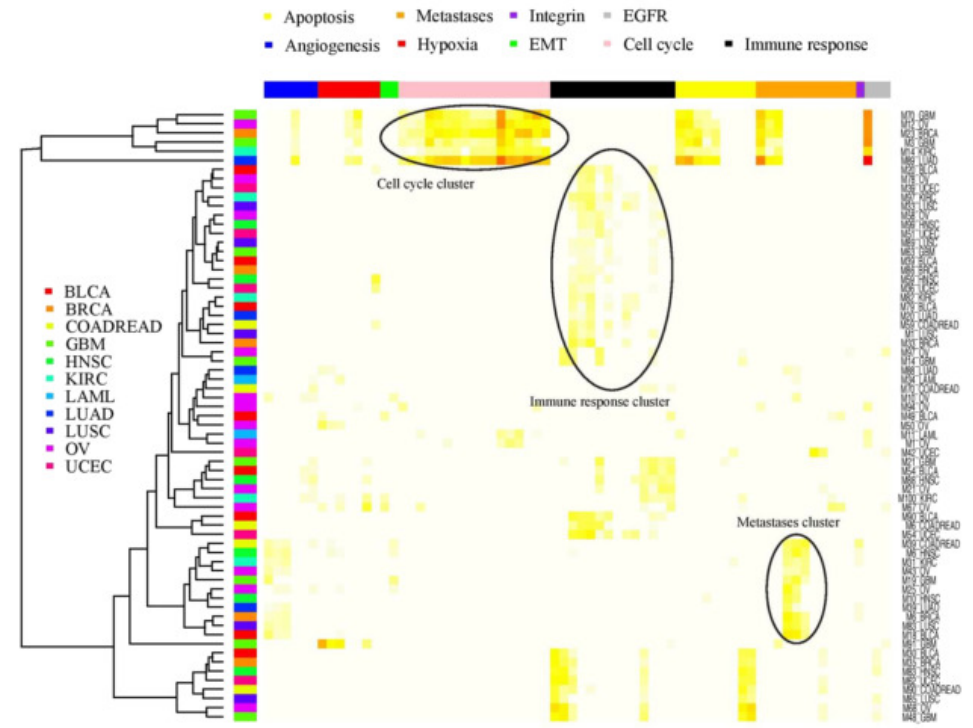


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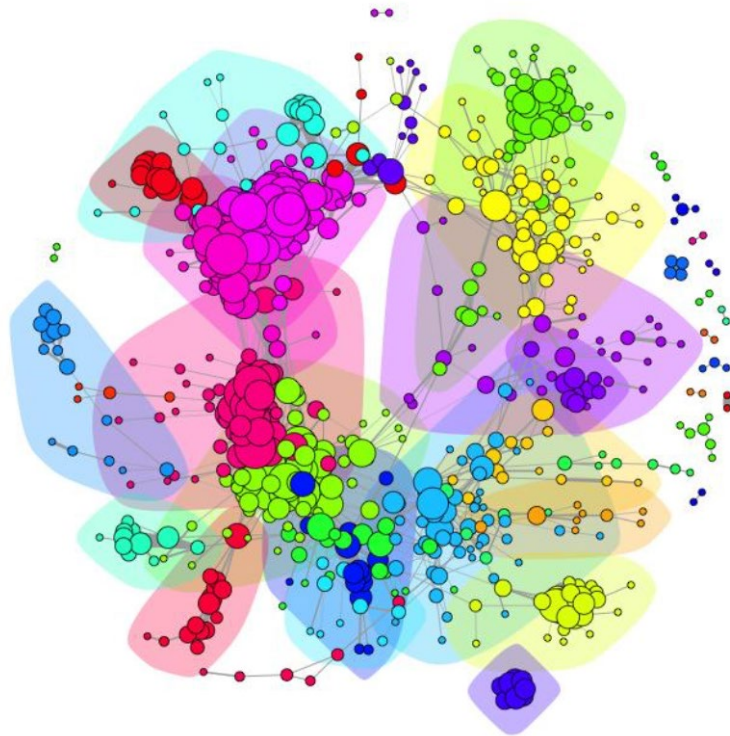


Pan-cancer functional categories

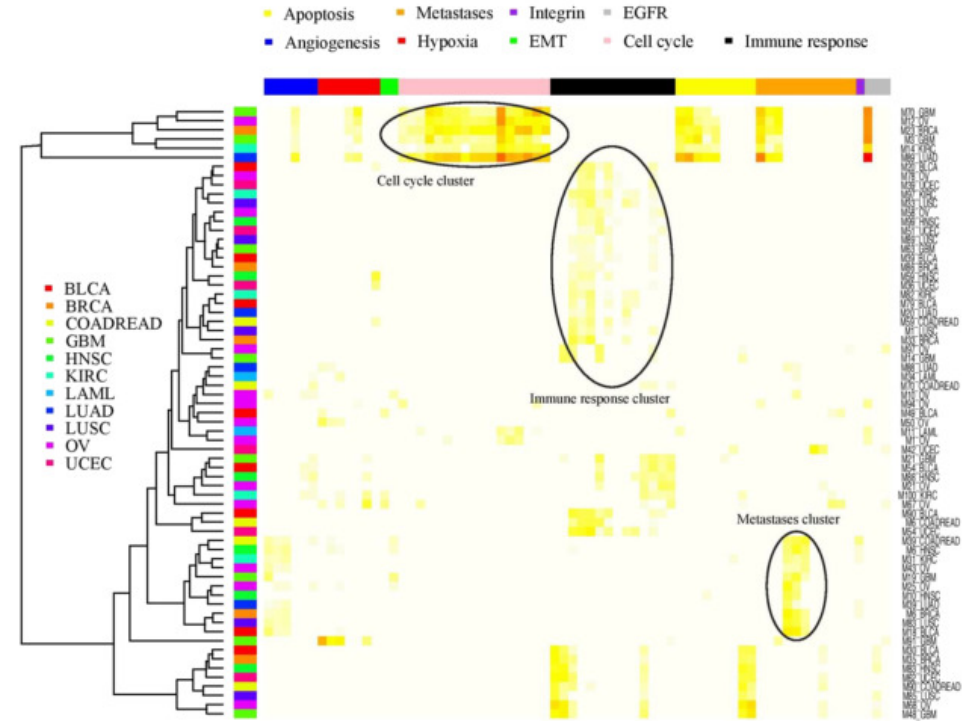


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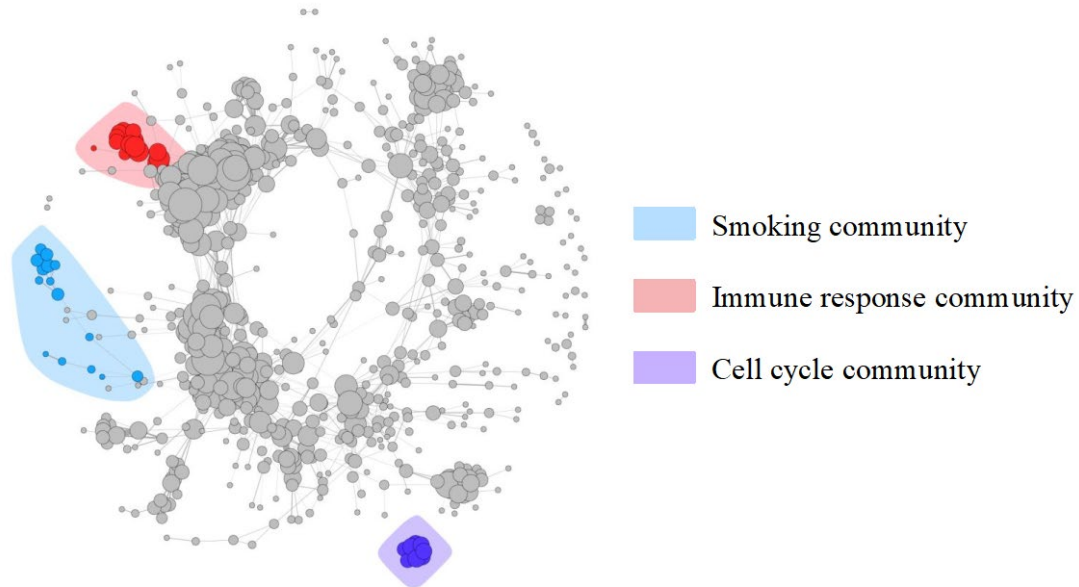
Pan-cancer functional categories



⇒ AMARETTO captures hallmarks of cancer

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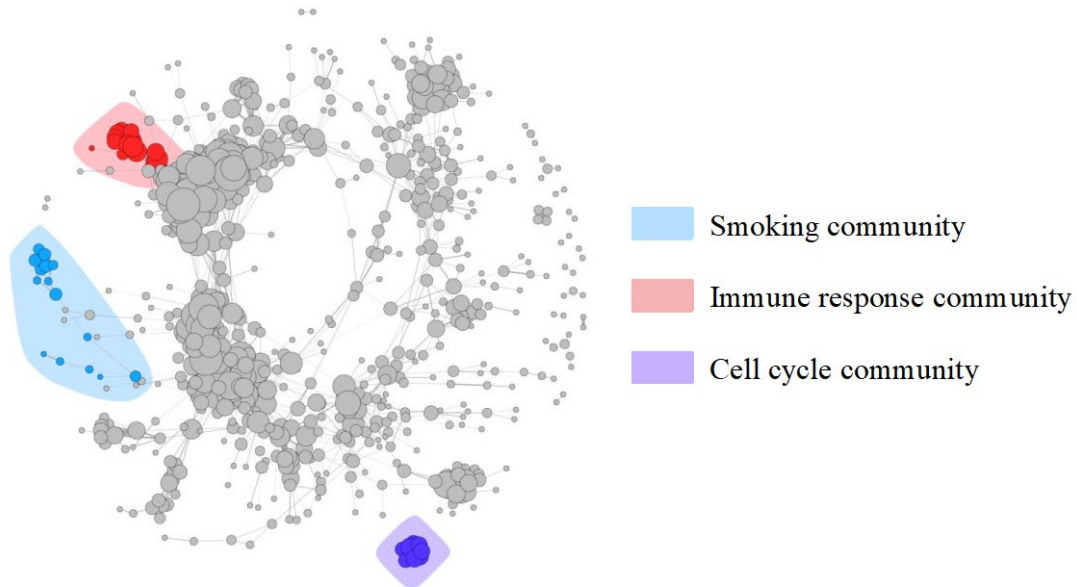
Driver discovery



- OAS2 pan-cancer driver of 'antiviral' interferon-modulated innate immune response
- GPX2 pan-cancer driver of smoking-induced cancer

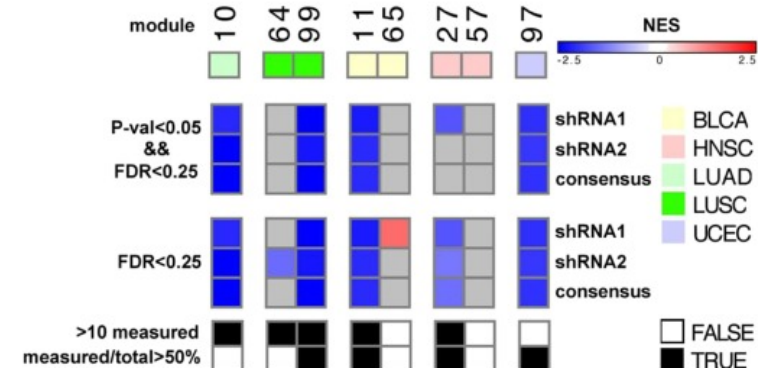
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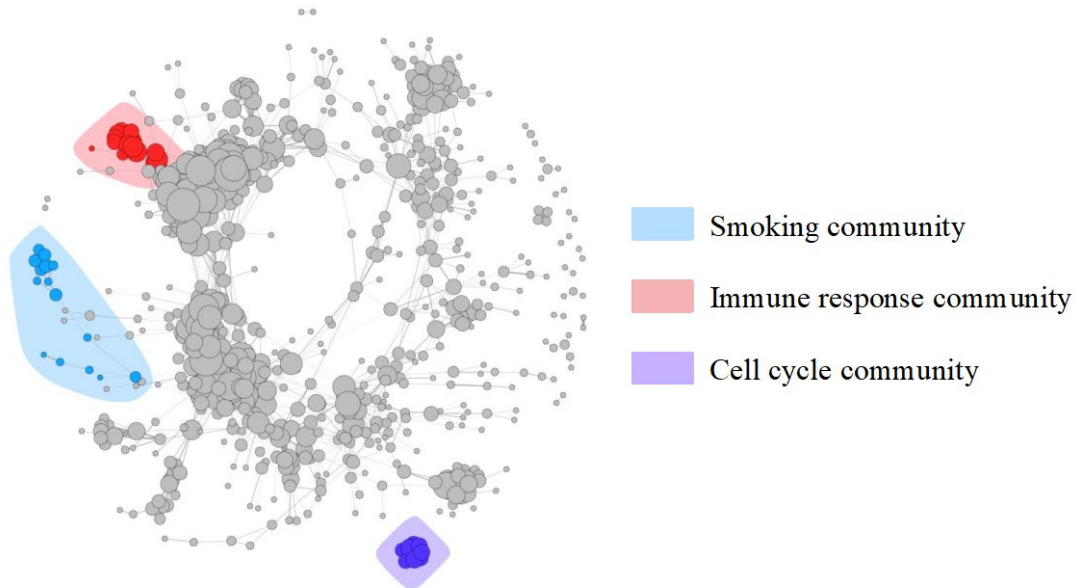
Driver validation



Genetic perturbation of GPX2 in the A549 (LUAD) cell line
 ⇒ Knocking down GPX2 represses target genes in GPX2-regulated modules

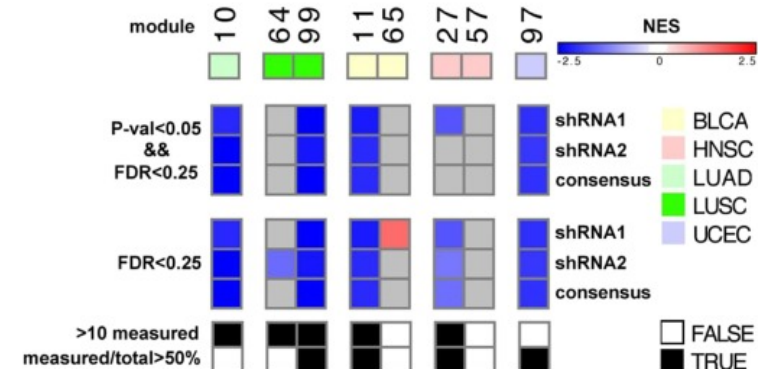
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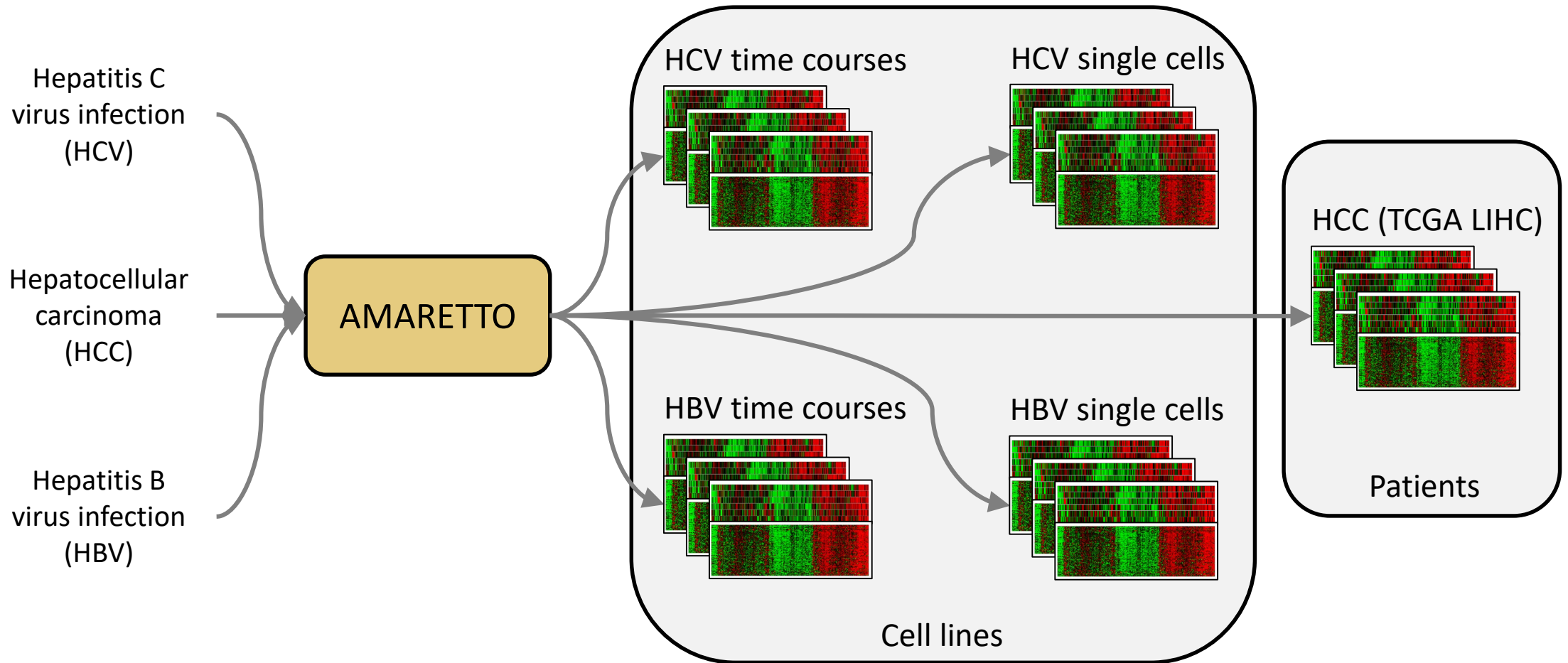


Genetic perturbation of GPX2 in the A549 (LUAD) cell line
 ⇒ Knocking down GPX2 represses target genes in GPX2-regulated modules

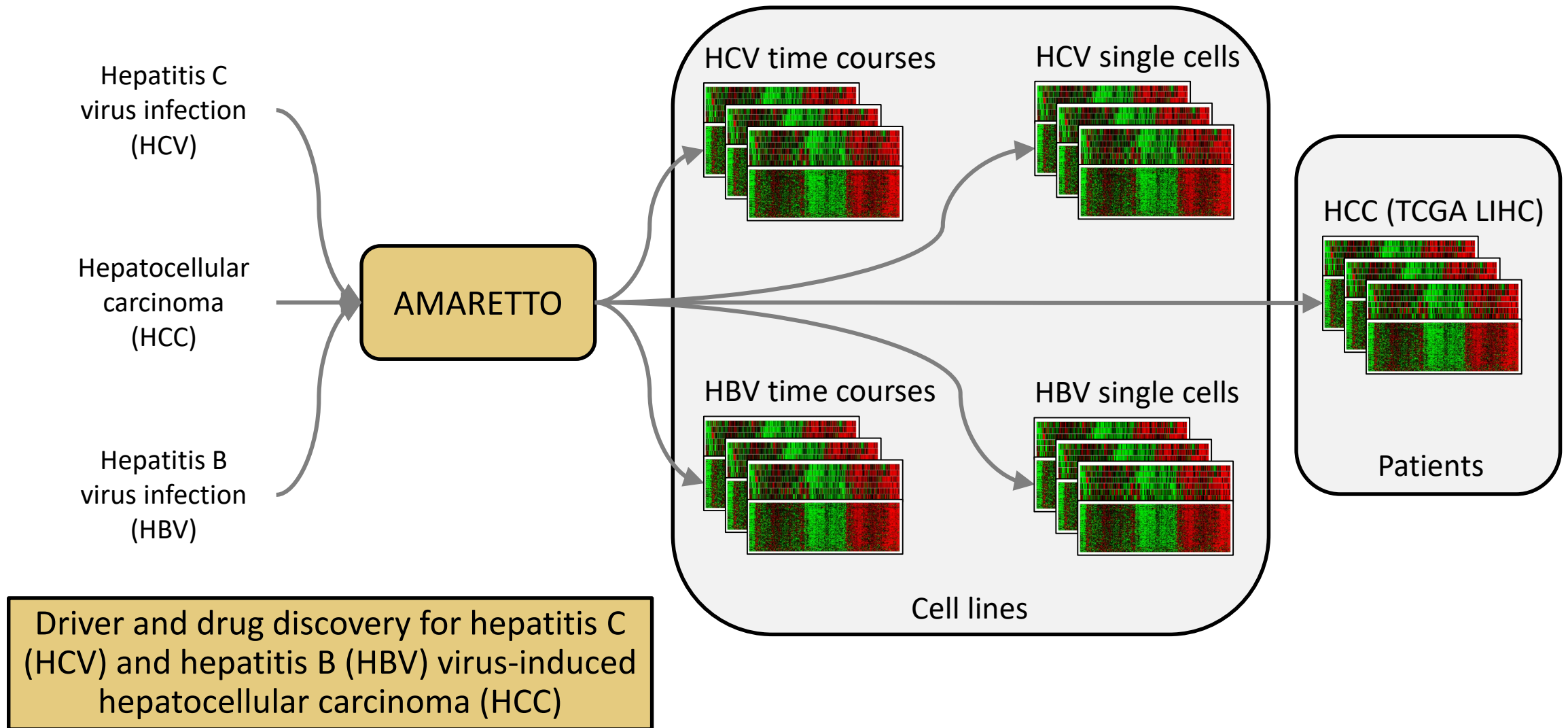
⇒ **AMARETTO facilitates identification of known and novel cancer drivers and their targets**

*AMARETTO application 2: virus-induced cancer

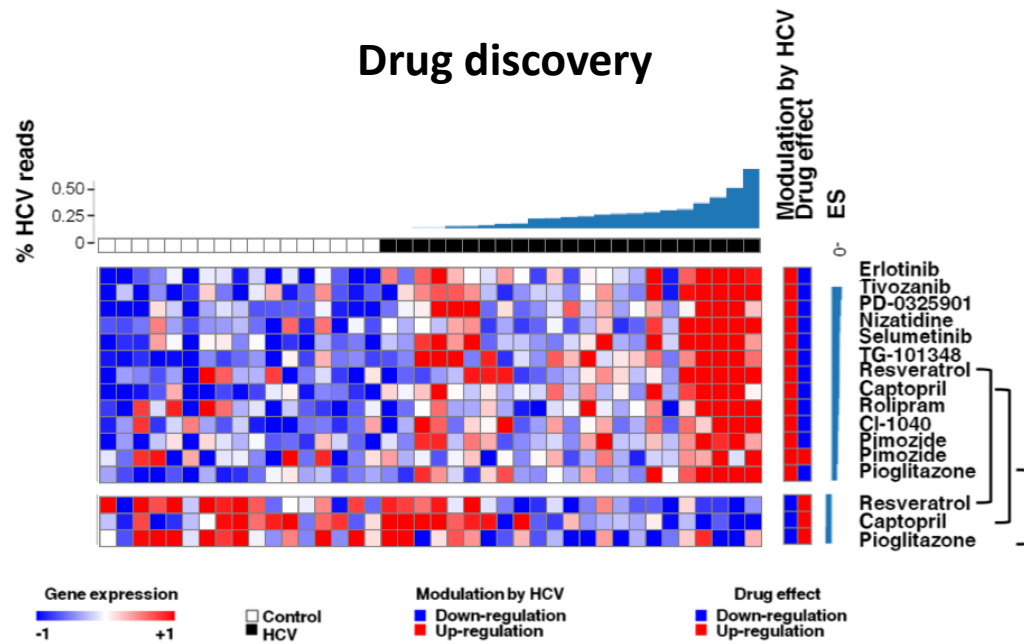
*AMARETTO application 2: virus-induced cancer



*AMARETTO application 2: virus-induced cancer



*AMARETTO application 2: virus-induced cancer

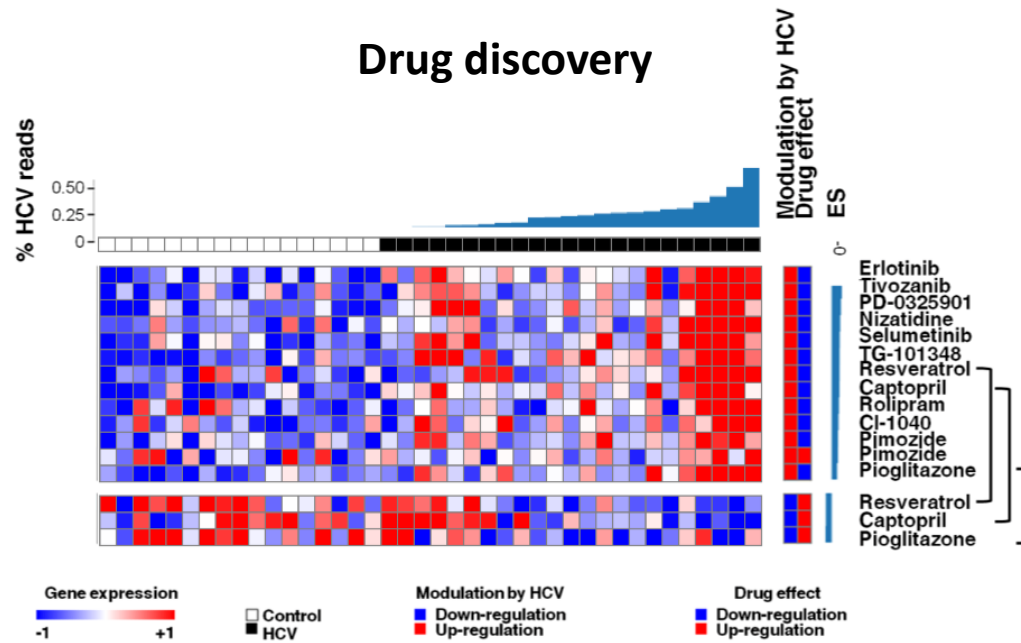


Chemical perturbations in cell lines

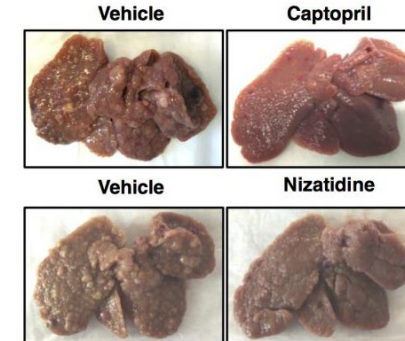
Predict which drugs can reverse disease-associated modules

Alternative treatments with less severe adverse effects

*AMARETTO application 2: virus-induced cancer



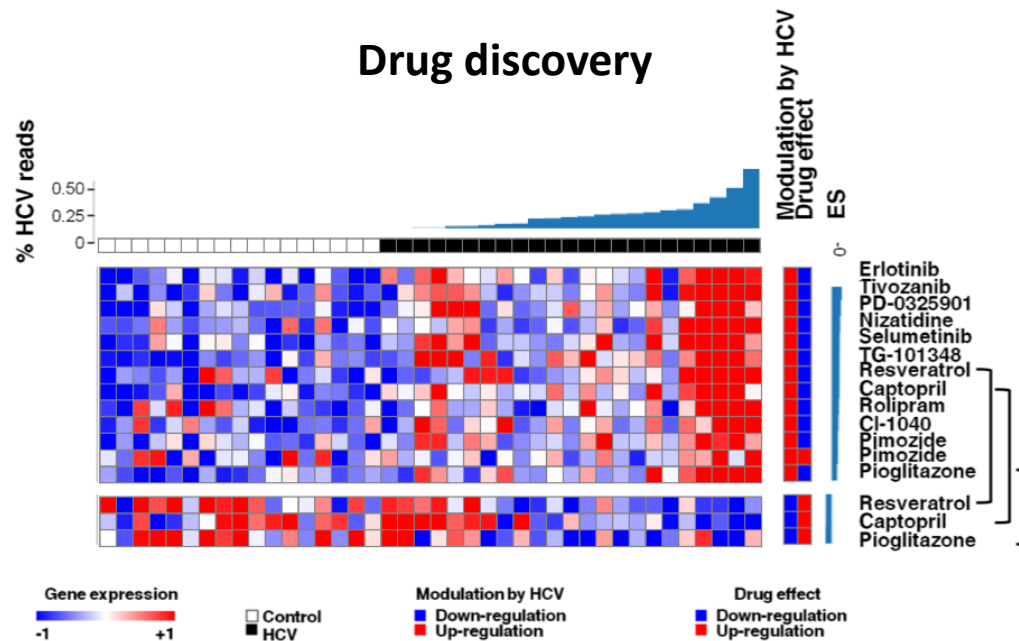
Drug validation



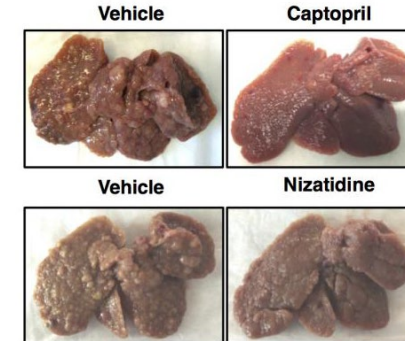
Chemical perturbations in cell lines
 Predict which drugs can reverse disease-associated modules
 Alternative treatments with less severe adverse effects

Experimental validation of drugs in rat models
 ⇒ Two novel compounds attenuate HCC development
 ⇒ Safe and low-cost approach for chemoprevention of HCC?

*AMARETTO application 2: virus-induced cancer



Drug validation

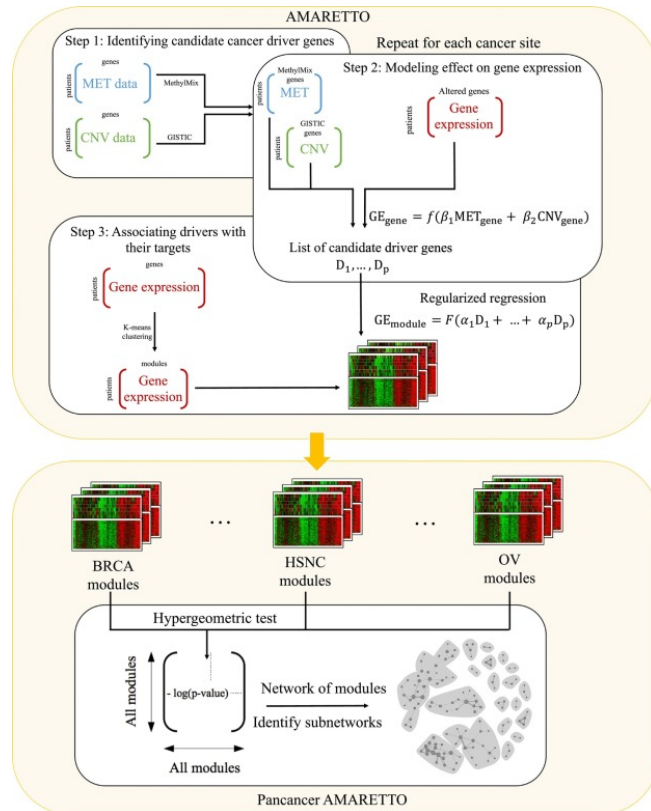


Chemical perturbations in cell lines
 Predict which drugs can reverse disease-associated modules
 Alternative treatments with less severe adverse effects

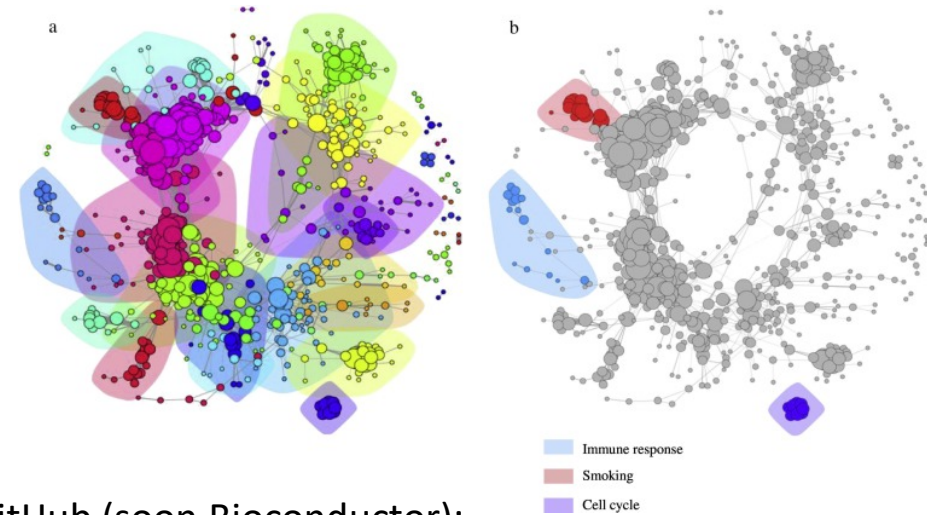
Experimental validation of drugs in rat models
 ⇒ Two novel compounds attenuate HCC development
 ⇒ Safe and low-cost approach for chemoprevention of HCC?

⇒ **AMARETTO facilitates identification of known and novel drug compounds and how they modulate cancer drivers and their targets**

*AMARETTO source code & analysis tools



Champion *et al.*, EBioMedicine 2018



R packages in GitHub (soon Bioconductor):

- <https://github.com/gevaertlab/AMARETTO>
- <https://github.com/broadinstitute/CommunityAMARETTO>

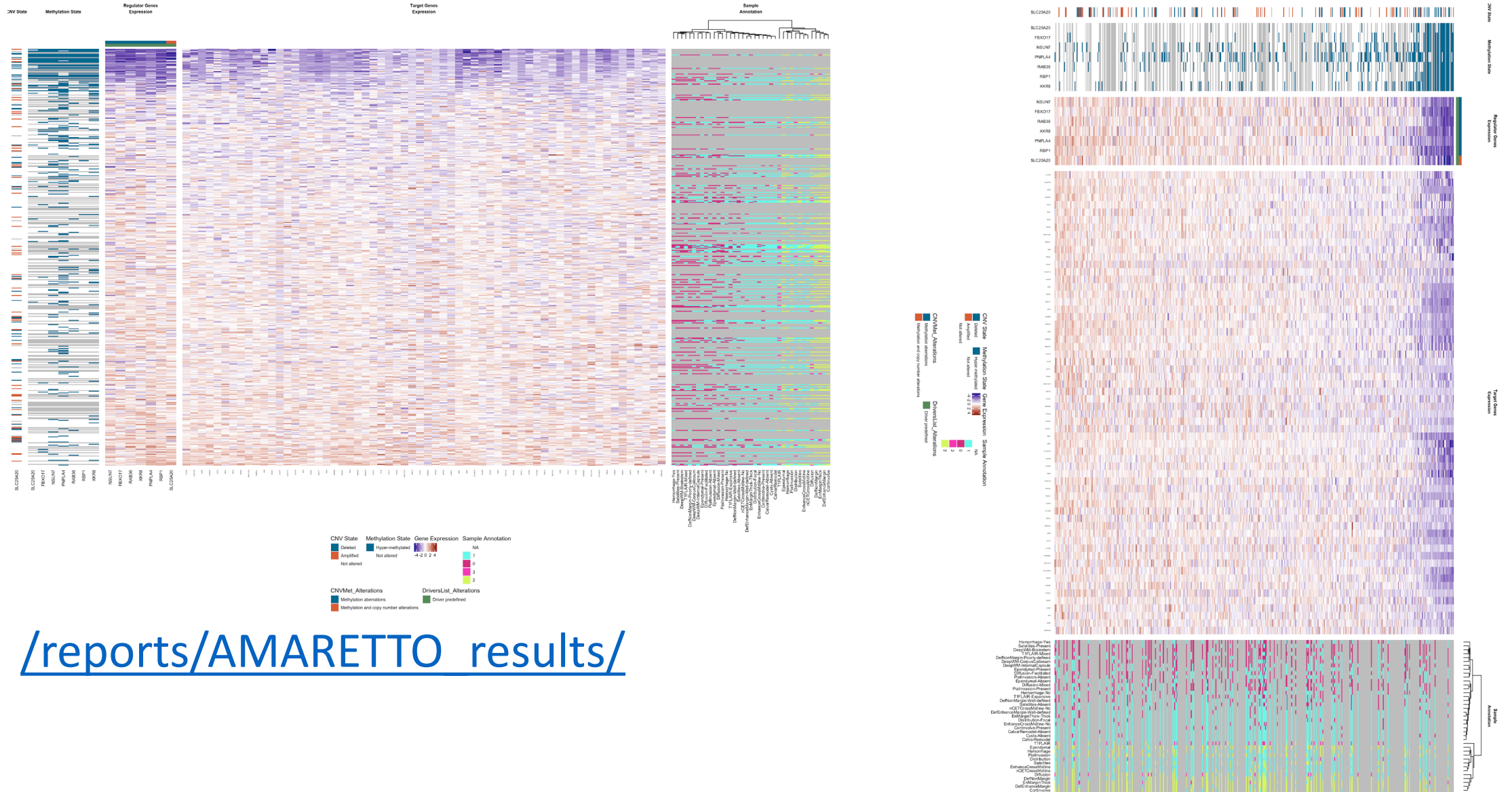
User-friendly analysis modules in GenePattern:

- <https://cloud.genepattern.org/module.analysis:00378>
- <https://cloud.genepattern.org/module.analysis:00380>

*AMARETTO:

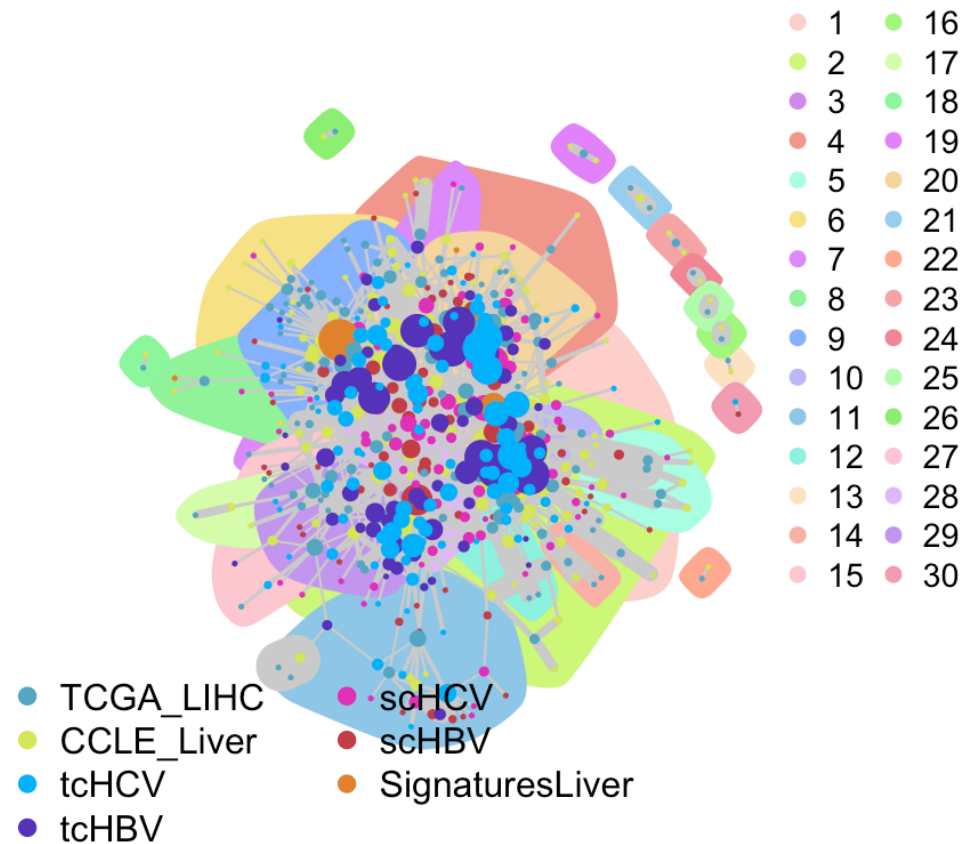
1. Captures hallmarks of cancer
2. Facilitates identification of known and novel cancer drivers and their targets
3. Facilitates identification of known and novel drug compounds and how they modulate cancer drivers and their targets

AMARETTO report: multi-omics & imaging data fusion in GBM



/reports/AMARETTO_results/

Community-AMARETTO report: HCV/HBV virus-induced HCC/LIHC



[/reports/Community-AMARETTO results/](/reports/Community-AMARETTO_results/)

AMARETTO module in GenePattern

(<https://cloud.genepattern.org/module.analysis:00378>)

GenePattern amaretto-team 0.0 KB / 30 GB

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Input data

expression file* **Drag Files Here** Batch ?
2GB file upload limit using the Upload File... button. For files > 2GB upload from the Files tab.

A gct file containing the gene expression profiles

copy number file **Drag Files Here** Batch ?
2GB file upload limit using the Upload File... button. For files > 2GB upload from the Files tab.

A gct file containing the copy number profiles

methylation file **Drag Files Here** Batch ?
2GB file upload limit using the Upload File... button. For files > 2GB upload from the Files tab.

A gct file containing the methylation profiles

driver gene list selection mode* Batch ?

Use the driver gene list file (if provided), compute a list from the CNV and/or MET data, or compute and intersect with a provided driver gene list

driver gene list* Batch ?

Predefined list of driver genes to use instead of or in addition to the list computed from CNV and/or Methylation data in a text file, one gene per line.

driver gene list file **Drag Files Here** Batch ?
2GB file upload limit using the Upload File... button. For files > 2GB upload from the Files tab.

A text file containing a list of driver genes to use instead of the predefined lists

AMARETTO module in GenePattern

(<https://cloud.genepattern.org/module.analysis:00378>)

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Input data

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Upload File... Add Path or URL... Drag Files Here

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A gct file containing the gene expression profiles

copy number file Batch ?

Upload File... Add Path or URL... Drag Files Here

2GB file upload limit using the Upload File... button. For files > 2GB upload from the Files tab.

A gct file containing the copy number profiles

methylation file Batch ?

Upload File... Add Path or URL... Drag Files Here

2GB file upload limit using the Upload File... button. For files > 2GB upload from the Files tab.

A gct file containing the methylation profiles

driver gene list selection mode* Batch ?

Use list computed from CNV/MET data

Use the driver gene list file (if provided), compute a list from the CNV and/or MET data, or compute and intersect with a provided driver gene list

driver gene list* Batch ?

MSigDB driver genes

Predefined list of driver genes to use instead of or in addition to the list computed from CNV and/or Methylation data in a text file, one gene per line.

driver gene list file Batch ?

Upload File... Add Path or URL... Drag Files Here

2GB file upload limit using the Upload File... button. For files > 2GB upload from the Files tab.

A text file containing a list of driver genes to use instead of the predefined lists

AMARETTO module in GenePattern

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Upload File... Add Path or URL... Drag Files Here

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A gct file containing the gene expression profiles

copy number file Batch ?

Upload File... Add Path or URL... Drag Files Here

2GB file upload limit using the Upload File... button. For files > 2GB upload from the Files tab.

A gct file containing the copy number profiles

methylation file Batch ?

Upload File... Add Path or URL... Drag Files Here

2GB file upload limit using the Upload File... button. For files > 2GB upload from the Files tab.

A gct file containing the methylation profiles

driver gene list selection mode* Batch ?

Use list computed from CNV/MET data

Use the driver gene list file (if provided), compute a list from the CNV and/or MET data, or compute and intersect with a provided driver gene list

driver gene list* Batch ?

MSigDB driver genes

Predefined list of driver genes to use instead of or in addition to the list computed from CNV and/or Methylation data in a text file, one gene per line.

driver gene list file Batch ?

Upload File... Add Path or URL... Drag Files Here

2GB file upload limit using the Upload File... button. For files > 2GB upload from the Files tab.

A text file containing a list of driver genes to use instead of the predefined lists

AMARETTO module in GenePattern

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Basic parameters

number of modules* Batch ?

Number of modules

percent genes* Batch ?

Percent genes to use

output file* Batch ?

Base name for output files

Hyper geometric test Batch ?

gene sets database* or Batch ?

Gene sets database from GSEA website. Upload a gene set if your gene set is not listed as a choice from MSigDB.

Job Options Batch ?

job memory Batch ?

walltime Batch ?

the runtime limit for the job in {days-hh:mm:ss} format

job cpuCount Batch ?

optional --container-overrides vcpus=(job.cpuCount)

AMARETTO module in GenePattern

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Basic parameters

number of modules* Batch ?

Number of modules

percent genes* Batch ?

Percent genes to use

output file* Batch ?

Base name for output files

Hyper geometric test

or Batch ?

gene sets database*

Gene sets database from GSEA website. Upload a gene set if your gene set is not listed as a choice from MSigDB.

Job Options

job memory Batch ?

walltime Batch ?

the runtime limit for the job in {days-hh:mm:ss} format

job cpuCount Batch ?

optional --container-overrides vcpus=(job.cpuCount)

AMARETTO module in GenePattern

(<https://cloud.genepattern.org/module.analysis:00378>)

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Basic parameters

number of modules* 10 Batch ?

Number of modules

percent genes* 5 Batch ?

Percent genes to use

output file* <expression.file_basename> Batch ?

Base name for output files

Hyper geometric test

Batch ?

gene sets database* Select a file or Upload your own file

c2.cp.v6.2.symbols.gmt [Curated]

Gene sets database from GSEA website. Upload a gene set if your gene set is not listed as a choice from MSigDB.

Job Options

job memory 2 Gb Batch ?

walltime short (2 hours) Batch ?

the runtime limit for the job in {days-hh:mm:ss} format

job cpuCount 4 Batch ?

optional --container-overrides vcpus=(job.cpuCount)

Community-AMARETTO module in GenePattern

(<https://cloud.genepattern.org/module.analysis:00380>)

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amaretto result files* Batch ?

Upload Files... Add Paths or URLs... Drag Files Here

2GB file upload limit using the Upload Files... button. For files > 2GB upload from the Files tab.

Files containing the zipped AMARETTO results

output file* Batch ?

CommunityAMARETTOResults

Name for output file

amaretto report files Batch ?

Upload Files... Add Paths or URLs... Drag Files Here

2GB file upload limit using the Upload Files... button. For files > 2GB upload from the Files tab.

Files containing the zipped AMARETTO reports with name prefixes matching the AMARETTO result files.

gene sets database* Batch ?

Select a file or Upload your own file

c2.all.v6.2.symbols.gmt [Curated]

Gene sets database from GSEA website. Upload a gene set if your gene set is not listed as a choice from MSigDB.

from msigdb* Batch ?

yes

For an uploaded geneset, are they MSigDB gene sets that should be linked to the MSigDB web site

gmt url present* Batch ?

yes

For an uploaded geneset, is there a link in the description (second) column to use in the report

Job Options

job memory Batch ?

2 Gb

walltime Batch ?

short (2 hours)

the runtime limit for the job in {days-hh:mm:ss} format

job cpuCount Batch ?

1

Community-AMARETTO module in GenePattern

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amaretto result files*

Upload Files... Add Paths or URLs... Drag Files Here

2GB file upload limit using the Upload Files... button. For files > 2GB upload from the Files tab.

Files containing the zipped AMARETTO results

output file* CommunityAMARETTOResults

Name for output file

amaretto report files

Upload Files... Add Paths or URLs... Drag Files Here

2GB file upload limit using the Upload Files... button. For files > 2GB upload from the Files tab.

Files containing the zipped AMARETTO reports with name prefixes matching the AMARETTO result files.

gene sets database* Select a file or Upload your own file

c2.all.v6.2.symbols.gmt [Curated]

Gene sets database from GSEA website. Upload a gene set if your gene set is not listed as a choice from MSigDB.

from msigdb* yes

For an uploaded geneset, are they MSigDB gene sets that should be linked to the MSigDB web site

gmt url present* yes

For an uploaded geneset, is there a link in the description (second) column to use in the report

Job Options

job memory 2 Gb

walltime short (2 hours)

the runtime limit for the job in {days-hh:mm:ss} format

job cpuCount 1

Community-AMARETTO module in GenePattern

(<https://cloud.genepattern.org/module.analysis:00380>)

The screenshot shows the GenePattern web interface for configuring the Community-AMARETTO module. The interface includes a top navigation bar with 'GenePattern' logo, user profile 'amaretto-team', and a storage indicator '0.0 KB / 30 GB'. A left sidebar contains navigation tabs for 'Modules', 'Jobs', and 'Files', along with search and module lists. The main area is a configuration form with several sections:

- amaretto result files***: A dashed box labeled 'Drag Files Here' with 'Upload Files...' and 'Add Paths or URLs...' buttons. Below it, a text input field contains 'CommunityAMARETTOResults'.
- output file***: A text input field with the value 'CommunityAMARETTOResults'.
- amaretto report files**: Another dashed box labeled 'Drag Files Here' with 'Upload Files...' and 'Add Paths or URLs...' buttons.
- gene sets database***: A section highlighted with a red box. It contains a 'Select a file' button, an 'or' label, and an 'Upload your own file' button. Below these is a dropdown menu showing 'c2.all.v6.2.symbols.gmt [Curated]'.
- from msigdb***: A dropdown menu set to 'yes'.
- gmt url present***: A dropdown menu set to 'yes'.
- Job Options**: A section with a blue header containing:
 - job memory**: A dropdown menu set to '2 Gb'.
 - walltime**: A dropdown menu set to 'short (2 hours)'.
 - job cpuCount**: A dropdown menu set to '1'.

Each configuration field has a 'Batch ?' button to its right. The 'gene sets database*' section is highlighted with a red border.

AMARETTO module in Github

(<https://github.com/gevaertlab/AMARETTO>)

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Regulatory network inference and driver gene evaluation using integrative multi-omics analysis and penalized regression

134 commits 4 branches 0 releases 7 contributors Apache-2.0

Branch: master New pull request Create new file Upload files Find file Clone or download

 monabiyan Bioconductor changes, optimizing code	Latest commit e2dca10 2 days ago
 AMARETTO_EXAMPLE	Bioconductor submission 16 days ago
 R	Bioconductor changes, optimizing code 2 days ago
 data	Bioconductor submission 16 days ago
 files	Bioconductor submission 17 days ago
 inst	Bioconductor submission 14 days ago
 man	Bioconductor submission 14 days ago
 vignettes	BioC changes 13 days ago
 .Rbuildignore	Bioconductor submission 15 days ago

Community-AMARETTO module in Github

(<https://github.com/broadinstitute/CommunityAMARETTO>)

The screenshot shows the GitHub repository page for `broadinstitute / CommunityAMARETTO`. The repository has 85 commits, 2 branches, 0 releases, and 4 contributors. The latest commit is by `monabiyan` with the message "memory overload issue is fixed." The repository structure includes folders `R`, `inst/templates`, `man`, and `src`, and files `.DS_Store`, `.Rbuildignore`, and `.gitignore`.

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No description, website, or topics provided. Edit

Manage topics

85 commits 2 branches 0 releases 4 contributors

Branch: master New pull request Create new file Upload files Find file Clone or download

`monabiyan` memory overload issue is fixed. Latest commit 85f7013 17 hours ago

R	memory overload issue is fixed.	17 hours ago
inst/templates	move legend slightly to left	2 months ago
man	GenePattern Changes	6 days ago
src	Build Rpackage structure	4 months ago
.DS_Store	eval function updated	12 days ago
.Rbuildignore	Build Rpackage structure	4 months ago
.gitignore	Output Community	2 months ago

Acknowledgements

Pochet Lab (BWH/HMS/Broad)

Mohsen Nabian

Celine Everaert

Rileen Sinha

Tom Croonenborghs

James Kozubek

Karun Kiani

Nikolaus Obholzer

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Vincent Carey

Gevaert Lab (Stanford/Broad)

Olivier Gevaert

Jayendra Ravindra Shinde

Shaimaa Hesham Bakr

Andrew Gentles

Kevin Brennan

Magali Champion

Hernaez Lab (Illinois)

Mikel Hernaez

Mesirov Lab (UCSD/Broad)

Jill Mesirov

Michael Reich

Ted Liefeld

Thorin Tabor

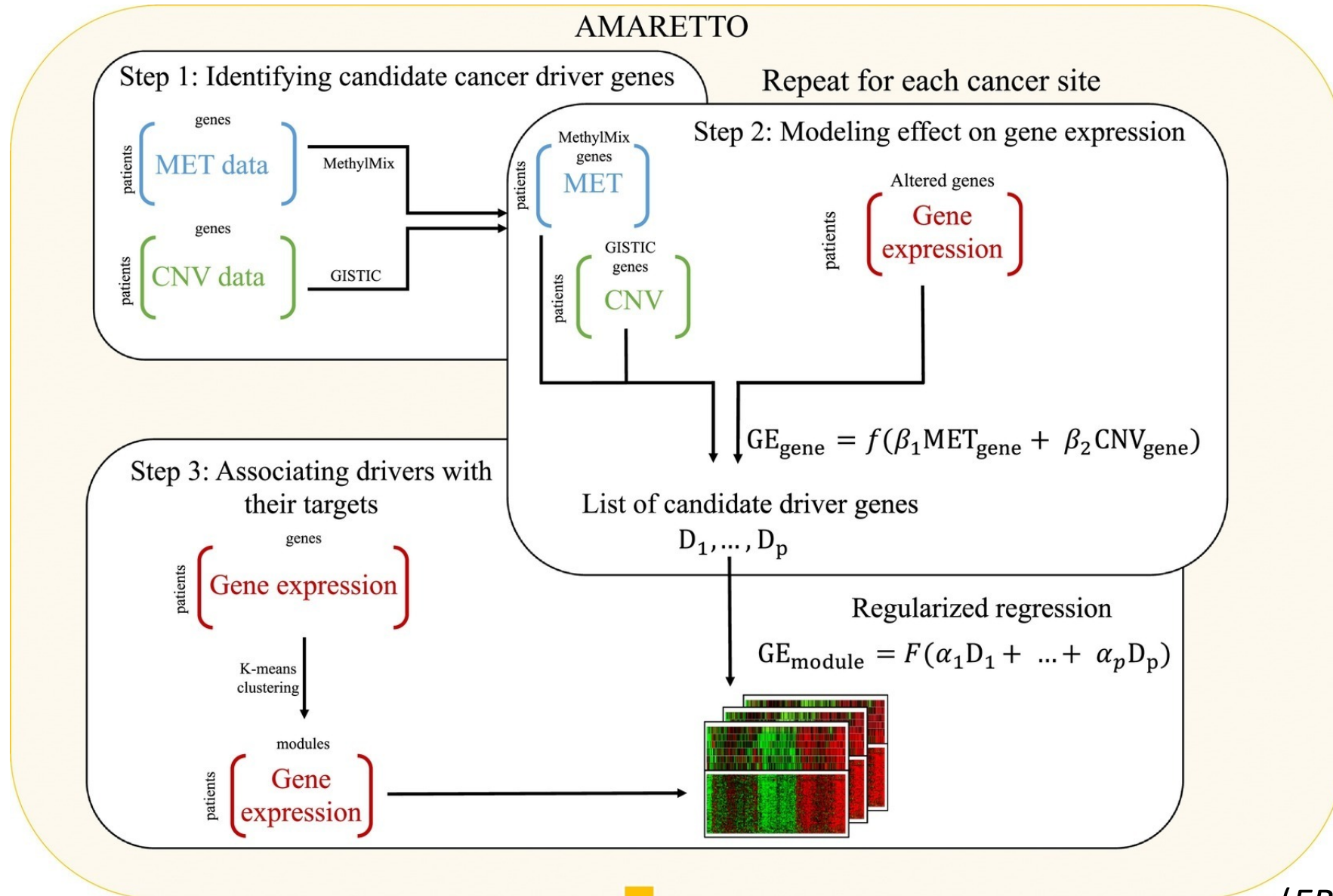
Baumert Lab (Strasbourg)

Thomas Baumert

Joachim Lupberger

Eloi Verrier

AMARETTO infers regulatory cell circuits – cancer drivers and their targets – via multi-omics data fusion



Community-AMARETTO learns communities across regulatory networks inferred from different resources

