Federated sharing and processing of genomic datasets for tertiary data analysis Arif Canakoglu, Pietro Pinoli, Andrea Gulino, Luca Nanni, Marco Masseroli, Stefano Ceri

Supplementary material

Federated GMQL queries

Here, we present the exact queries that we introduced in the main manuscript and the execution log of the BEST query. All the queries are ready to be used on the dedicated server (GeCo as LOCAL). We present 4 distributed strategies (DIST-1 to DIST-4), 3 centralized ones (CENT-1 to CENT-3), and the BEST strategy, which have been discussed in the main manuscript. We excluded the externalized strategy (EXT), because the AWS instances are accessible only on demand.

DIST-1:

Distributed query 1: In this example, all the unary operations are on the machine where the dataset is selected. The binary operations, JOIN and MAP, are both executed on the DEIB instance.

```
CINECA.HG19 TCGA rnaseqv2 gene;
# 2
AccExp = COVER(1, ANY; aggregate: mean exp as AVG(normalized count); at:CINECA)
AccExpFilt = SELECT(region: mean exp > 1000; at:CINECA) AccExp;
Myc = SELECT(gcm curated cell line == "H1-hESC" AND
         target name == "MYC-human" AND
         file output type == "conservative idr thresholded peaks"; at:DEIB)
                                       DEIB.HG19 ENCODE NARROW 2019 01;
GeneMyc = JOIN(dist < 0; output: left distinct; at:DEIB) AccExpFilt Myc;</pre>
myMutation = SELECT(at:LOCAL) myMutation;
myMutationMerge = MERGE(at:LOCAL) myMutation;
GeneMycMut= MAP(count name: mut count; at:DEIB) GeneMyc myMutationMerge;
ResGenes = SELECT(region:mut_count > 0; at:DEIB) GeneMycMut;
MATERIALIZE ResGenes INTO ResGenes;
```

DIST-2:

Distributed query 2: In this example, all the unary operations are on the machine where the dataset is selected. The binary operations, JOIN and MAP, are both executed on the CINECA instance.

```
AccRnaseq = SELECT (manually_curated__tumor_tag == "acc" AND manually_curated__tissue_status == "tumoral"; at:CINECA)
                                            CINECA.HG19 TCGA rnaseqv2 gene;
AccExp = COVER(1, ANY; aggregate: mean exp as AVG(normalized count); at:CINECA)
AccRnaseq;
AccExpFilt = SELECT(region: mean exp > 1000; at:CINECA) AccExp;
Myc = SELECT(gcm_curated__cell_line == "H1-hESC" AND
           target name == "MYC-human" AND
           file__output_type == "conservative idr thresholded peaks"; at:DEIB)
                                           DEIB.HG19 ENCODE NARROW 2019 01;
GeneMyc = JOIN(dist < 0; output: left distinct; at:CINECA) AccExpFilt Myc;</pre>
myMutation = SELECT(at:LOCAL) myMutation;
myMutationMerge = MERGE(at:LOCAL) myMutation;
GeneMycMut= MAP(count name: mut count; at:CINECA) GeneMyc myMutationMerge;
ResGenes = SELECT(region:mut count > 0; at:CINECA) GeneMycMut;
MATERIALIZE ResGenes INTO ResGenes;
```

DIST-3:

Distributed query 3: In this example, all the unary operations are on the machine where the dataset is selected. The binary operations, JOIN and MAP, are executed on the DEIB and GeCo (LOCAL) instance, respectively.

```
AccRnaseg = SELECT (manually curated tumor tag == "acc" AND
                manually_curated__tissue_status == "tumoral"; at:CINECA)
                                          CINECA.HG19 TCGA rnaseqv2 gene;
# 2
AccExp = COVER(1, ANY; aggregate: mean exp as AVG(normalized count); at:CINECA)
AccRnaseq;
AccExpFilt = SELECT(region: mean exp > 1000; at:CINECA) AccExp;
Myc = SELECT(gcm_curated__cell_line == "H1-hESC" AND
           target__name == "MYC-human" AND
           file output type == "conservative idr thresholded peaks"; at:DEIB)
                                            DEIB.HG19 ENCODE NARROW 2019 01;
GeneMyc = JOIN(dist < 0; output: left_distinct; at:DEIB) AccExpFilt Myc;</pre>
myMutation = SELECT(at:LOCAL) myMutation;
myMutationMerge = MERGE(at:LOCAL) myMutation;
GeneMycMut= MAP(count name: mut count; at:LOCAL) GeneMyc myMutationMerge;
ResGenes = SELECT(region:mut count > 0; at:LOCAL) GeneMycMut;
MATERIALIZE ResGenes INTO ResGenes;
```

DIST-4:

Distributed query 4: In this example, all the unary operations are on the machine where the dataset is selected. The binary operations, JOIN and MAP, are executed on the CINECA and GeCo (LOCAL) instances, respectively.

```
AccRnaseq = SELECT(manually curated tumor tag == "acc" AND
                manually_curated__tissue_status == "tumoral"; at:CINECA)
                                         CINECA.HG19 TCGA rnaseqv2 gene;
# 2
AccExp = COVER(1, ANY; aggregate: mean exp as AVG(normalized count); at:CINECA)
AccRnaseq;
AccExpFilt = SELECT(region: mean exp > 1000; at:CINECA) AccExp;
Myc = SELECT(gcm_curated__cell_line == "H1-hESC" AND
           target_ name == "MYC-human" AND
           file output type == "conservative idr thresholded peaks"; at:DEIB)
                                           DEIB.HG19 ENCODE NARROW 2019 01;
GeneMyc = JOIN(dist < 0; output: left_distinct; at:CINECA) AccExpFilt Myc;</pre>
myMutation = SELECT(at:GeCo ) myMutation;
myMutationMerge = MERGE(at:LOCAL) myMutation;
GeneMycMut= MAP(count name: mut count; at:LOCAL) GeneMyc myMutationMerge;
ResGenes = SELECT(region:mut count > 0; at:LOCAL) GeneMycMut;
MATERIALIZE ResGenes INTO ResGenes;
```

CENT-1:

Centralized query 1: In this example, all the selection operations run on the machine where the dataset is selected. All the others run on DEIB instance.

```
AccRnaseq = SELECT(manually_curated__tumor_tag == "acc" AND
                manually_curated__tissue_status == "tumoral"; at:CINECA)
                                           CINECA.HG19 TCGA rnaseqv2 gene;
AccExp = COVER(1, ANY; aggregate: mean exp as AVG(normalized count); at:DEIB) AccRnaseq;
AccExpFilt = SELECT(region: mean exp > 1000; at:DEIB) AccExp;
Myc = SELECT(gcm_curated__cell_line == "H1-hESC" AND
           target name == "MYC-human" AND
           file__output_type == "conservative idr thresholded peaks"; at:DEIB)
                                             DEIB.HG19 ENCODE NARROW 2019 01;
GeneMyc = JOIN(dist < 0; output: left distinct; at:DEIB) AccExpFilt Myc;</pre>
myMutation = SELECT(at:LOCAL) myMutation;
myMutationMerge = MERGE(at:DEIB) myMutation;
GeneMycMut= MAP(count name: mut count; at:DEIB) GeneMyc myMutationMerge;
ResGenes = SELECT(region:mut_count > 0; at:DEIB) GeneMycMut;
# 10
MATERIALIZE ResGenes INTO ResGenes;
```

CENT-2:

Centralized query 2: In this example, all the selection operations run on the machine where the dataset is selected. All the others run on CINECA instance.

```
AccRnaseq = SELECT(manually_curated__tumor_tag == "acc" AND
                manually_curated__tissue_status == "tumoral"; at:CINECA)
                                           CINECA.HG19 TCGA rnaseqv2 gene;
# 2
AccExp = COVER(1, ANY; aggregate: mean exp as AVG(normalized count); at:CINECA)
AccRnaseq;
AccExpFilt = SELECT(region: mean exp > 1000; at:CINECA) AccExp;
Myc = SELECT(gcm curated cell line == "H1-hESC" AND
           target name == "MYC-human" AND
           file_output_type == "conservative idr thresholded peaks"; at:DEIB)
                                              DEIB.HG19 ENCODE NARROW 2019 01;
GeneMyc = JOIN(dist < 0; output: left distinct; at:CINECA) AccExpFilt Myc;</pre>
myMutation = SELECT(at:LOCAL) myMutation;
myMutationMerge = MERGE(at:CINECA) myMutation;
GeneMycMut= MAP(count name: mut count; at:CINECA) GeneMyc myMutationMerge;
ResGenes = SELECT(region:mut count > 0; at:CINECA) GeneMycMut;
# 10
MATERIALIZE ResGenes INTO ResGenes;
```

CENT-3:

Centralized query 3: In this example, all the selection operations run on the machine where the dataset is selected. All the others run on GeCo (LOCAL) instance.

```
AccRnaseq = SELECT(manually_curated__tumor_tag == "acc" AND
                manually_curated__tissue_status == "tumoral"; at:CINECA)
                                            CINECA.HG19 TCGA rnaseqv2 gene;
AccExp = COVER(1, ANY; aggregate: mean exp as AVG(normalized count); at:LOCAL) AccRnaseq;
AccExpFilt = SELECT(region: mean exp > 1000; at:LOCAL) AccExp;
Myc = SELECT(gcm_curated__cell_line == "H1-hESC" AND
           target name == "MYC-human" AND
           file__output_type == "conservative idr thresholded peaks"; at:DEIB)
                                             DEIB.HG19 ENCODE NARROW 2019 01;
GeneMyc = JOIN(dist < 0; output: left distinct; at:LOCAL) AccExpFilt Myc;</pre>
myMutation = SELECT(at:LOCAL) myMutation;
myMutationMerge = MERGE(at:LOCAL) myMutation;
GeneMycMut= MAP(count name: mut count; at:LOCAL) GeneMyc myMutationMerge;
ResGenes = SELECT(region:mut_count > 0; at:LOCAL) GeneMycMut;
# 10
MATERIALIZE ResGenes INTO ResGenes;
```

BEST:

Best query: In this example, all the selection operations run on the machine where the dataset is selected, and also the cover operation run on CINECA instance, i.e., where the covered dataset is selected. All the others run on GeCo (LOCAL) instance.

```
AccRnaseg = SELECT (manually curated tumor tag == "acc" AND
                 manually_curated__tissue_status == "tumoral"; at:CINECA)
                                            CINECA.HG19 TCGA rnaseqv2 gene;
# 2
AccExp = COVER(1, ANY; aggregate: mean exp as AVG(normalized count); at:CINECA)
AccRnaseq;
AccExpFilt = SELECT(region: mean exp > 1000; at:LOCAL) AccExp;
Myc = SELECT(gcm_curated__cell_line == "H1-hESC" AND
           target__name == "MYC-human" AND
           file output type == "conservative idr thresholded peaks"; at:DEIB)
                                              DEIB.HG19 ENCODE NARROW 2019 01;
GeneMyc = JOIN(dist < 0; output: left_distinct; at:LOCAL) AccExpFilt Myc;</pre>
myMutation = SELECT(at:LOCAL) myMutation;
myMutationMerge = MERGE(at:LOCAL) myMutation;
GeneMycMut= MAP(count name: mut count; at:LOCAL) GeneMyc myMutationMerge;
ResGenes = SELECT(region:mut count > 0; at:LOCAL) GeneMycMut;
MATERIALIZE ResGenes INTO ResGenes;
```

The log file of run of the BEST execution

```
2019-07-29 15:49:38,350 Starting Federated query job canakoglu best 20190729 154937
2019-07-29 15:49:38,350 Splitting the computation DAG
2019-07-29 15:49:38,359 Getting DAGs to execute remotely
2019-07-29 15:49:38,363 Starting the federated query
2019-07-29 15:49:38,387 Sending sub-query to CINECA
2019-07-29 15:50:34,404 Execution time at remote (CINECA): 56 s.
2019-07-29 15:50:34,404 Moving temp_0 (metadata) from CINECA to LOCAL
2019-07-29 15:50:35,427 Execution time of moving from CINECA to LOCAL: 1 s.
2019-07-29 15:50:35,450 Sending sub-query to CINECA
2019-07-29 15:55:16,591 Execution time at remote (CINECA): 281s.
2019-07-29 15:55:16,591 Moving temp 1 (region) from CINECA to LOCAL
2019-07-29 15:55:19,616 Execution time of moving from CINECA to LOCAL: 3 s.
2019-07-29 15:55:19,638 Sending sub-query to DEIB
2019-07-29 15:55:58,969 Execution time at remote (DEIB): 39s.
2019-07-29 15:55:58,969 Moving temp 2 (metadata) from DEIB to LOCAL
2019-07-29 15:55:59,990 Execution time of moving from DEIB to LOCAL: 1 s.
2019-07-29 15:56:00,011 Sending sub-query to DEIB
2019-07-29 15:56:46,803 Execution time at remote (DEIB): 46s.
2019-07-29 15:56:46,803 Moving temp 3 (region) from DEIB to LOCAL
2019-07-29 15:56:47,827 Execution time of moving from DEIB to LOCAL: 1 s.
2019-07-29 15:56:47,828 Executing local query
2019-07-29 15:57:32,025 Execution time at local: 44 s.
2019-07-29 15:57:32,025 Total response time: 473 s.
```