Guide for trident v1.4.1.0

2

	$\boldsymbol{\alpha}$		1 -	1	
3	\cup (on	\mathbf{te}	nı	ιs

4	1	Inst	allation	1	
5	2	The	e trident CLI	2	
6		2.1	General notes	4	
7			2.1.1 Logging and command line output	4	
8			2.1.2 Package duplicates and versions	4	
9			2.1.3 Individual/Sample duplicates	4	
10			2.1.4 Group names in .fam files	5	
11			2.1.5 Whitespaces in the .janno file	5	
12	3	Pac	kage creation and manipulation commands	5	
13		3.1	Init command	5	
14		3.2	Fetch command	7	
15		3.3	Forge command	8	
16			3.3.1 The forge selection language	11	
17			3.3.2 Treatment of the genotype data while merging	12	
18			3.3.3 Treatment of the .janno file while merging	13	
19			3.3.4 Treatment of the .ssf file while merging	14	
20			3.3.5 Treatment of the .bib file while merging	14	
21			3.3.6 Other options	14	
22		3.4	Genoconvert command	15	
23		3.5	Jannocoalesce command	16	
24		3.6	Rectify command	18	
25	4	Insp	pection commands	19	
26		4.1	List command	19	
27		4.2	Summarise command	20	
28		4.3	Survey command		
29		4.4	Validate command	21	

1 Installation

See the Poseidon website (https://www.poseidon-adna.org/#/trident) or the GitHub repository (https://github.com/poseidon-framework/poseidon-hs) for up-to-date installation instructions.

2 The trident CLI

- Trident is a command line software tool structured in multiple subcommands. If you installed it properly you
- 25 can call it on the command line by typing trident. This will show an overview of the general options and all
- 36 subcommands, which are explained in detail below.

Usage: trident [--version] [--logMode MODE | --debug] [--errLength INT]

[--inPlinkPopName MODE] (COMMAND | COMMAND)

trident is a management and analysis tool for Poseidon packages. Report issues

here: https://github.com/poseidon-framework/poseidon-hs/issues

Available options:

-h,--help Show this help text
--version Show version number

--logMode MODE How information should be reported: NoLog, SimpleLog,

DefaultLog, ServerLog or VerboseLog.

(default: DefaultLog)

--debug Short for --logMode VerboseLog.

--errLength INT After how many characters should a potential error

message be truncated. "Inf" for no truncation.

(default: CharCount 1500)

--inPlinkPopName MODE Where to read the population/group name from the FAM

file in Plink-format. Three options are possible:

asFamily (default) | asPhenotype | asBoth.

Package creation and manipulation commands:

init Create a new Poseidon package from genotype data fetch Download data from a remote Poseidon repository forge Select packages, groups or individuals and create a

new Poseidon package from them

genoconvert Convert the genotype data in a Poseidon package to a

different file format

jannocoalesce Coalesce information from one or multiple janno files

to another one

rectify Adjust POSEIDON.yml files automatically to package

changes

Inspection commands:

list List packages, groups or individuals from local or

 ${\tt remote\ Poseidon\ repositories}$

summarise Get an overview over the content of one or multiple

Poseidon packages

survey Survey the degree of context information completeness

for Poseidon packages

validate Check Poseidon packages or package components for

structural correctness

trident allows to work directly with genotype data (see -p below), but it is optimized for the interaction
with Poseidon packages, which wrap and contextualize the data. Most trident subcommands therefore have a
central parameter, called --baseDir or simply -d to specify one or more base directories to look for packages.
For example, if all Poseidon packages live inside a repository at /path/to/poseidon/packages you would
simply say trident <subcommand> -d /path/to/poseidon/dirs/ and trident would automatically search
all subdirectories inside of the repository for valid Poseidon packages (as identified by valid POSEIDON.yml
files).

44 You can arrange a Poseidon repository in a hierarchical way. For example:

This structure then allows to select only the level of packages you are interested in, even individual ones. -d
can be given multiple times, which is particularly useful as you may have your own data to co-analyse with
external reference data. In this case you simply need to provide your own genotype data as yet another Poseidon
package to be added to your trident command. For example, you may have genotype data in EIGENSTRAT
format (trident supports EIGENSTRAT and PLINK as formats.):

```
~/my_project/my_project.geno
~/my_project/my_project.snp
~/my_project/my_project.ind
```

Then you can transform that into a skeleton Poseidon package with the init command. You can also do it manually by simply adding a POSEIDON.yml file, with, for example, the following content:

```
poseidonVersion: 2.7.1
title: My_awesome_project
description: Unpublished genetic data from my awesome project
contributor:
    - name: Stephan Schiffels
        email: schiffels@institute.org
packageVersion: 0.1.0
lastModified: 2020-10-07
genotypeData:
    format: EIGENSTRAT
    genoFile: my_project.geno
    snpFile: my_project.snp
    indFile: my_project.ind
```

```
jannoFile: my_project.janno
bibFile: sources.bib
```

- Two remarks: 1) All file paths in this POSEIDON.yml file are considered *relative* to the directory in which POSEIDON.yml resides. For this example we assume that this file is added into the same directory as the three genotype files. 2) Besides the genotype data files there are two (technically optional) files referenced in this example: sources.bib and my_project.janno. Of course you can add them manually init automatically creates empty dummy versions.
- Once you have set up your own Poseidon package (which is really only a skeleton so far), you can add it to your trident analysis, by simply adding your project directory to the command using -d, for example:

```
trident list -d /path/to/poseidon/packages/modern \
  -d /path/to/poseidon/packages/ReferenceGenomes \
  -d ~/my_project \
  --packages
```

$_{59}$ 2.1 General notes

63

67

68

72

73

80

82

60 2.1.1 Logging and command line output

- For all subcommands the general argument --logMode defines how trident reports messages (to stderr) on the command line:
 - NoLog: Hides all messages.
 - SimpleLog: Plain and simple output.
- DefaultLog: Adds the severity indicators (log levels) Info, Warning and Error before each message. This is the default setting.
 - ServerLog: Additionally adds timestamps before each message.
 - VerboseLog: Shows not just messages on the log levels Info, Warning and Error like the other modes, but also on the more verbose level Debug. Use this mostly relevant for debugging.
- 70 --debug is short for --logMode VerboseLog to activate this important log level more easily.

71 2.1.2 Package duplicates and versions

- For trident multiple packages in a set of base directories can share the same title, if they have different packageVersion numbers. If the version numbers are also identical or missing, then trident stops with an exception.
- The trident subcommands genoconvert, list, rectify, survey and validate by default consider all versions of each Poseidon package in the given base directories. The --onlyLatest flag causes them to instead only consider the latest versions.
- fetch and forge generally consider all package versions. Their selection language (see below) allows for detailed version handling.
 - summarize and jannocoalesce consider always only the latest package versions.

2.1.3 Individual/Sample duplicates

• Poseidon_IDs (so individual/sample names) within one package have to be unique, or trident will stop.

- We also discourage sample duplicates across packages in package repositories, but trident will generally
 continue with them. validate will fail though, if the --ignoreDuplicates flag is not set.
 - forge offers a special mechanism to resolve sample duplicates within its selection language.

$_{66}$ 2.1.4 Group names in .fam files

83

84

85

- The .fam file of PLINK-formatted genotype data is used inconsistently across different popular aDNA software tools to store group/population name information. The (global) trident option --inPlinkPopName with the arguments asFamily (default), asPhenotype and asBoth allows to control the reading of the population name from PLINK .fam files. The subcommands that write genotype data (forge, genoconvert) have a corresponding option --outPlinkPopName to specify this for the output.
- 92 2.1.5 Whitespaces in the .janno file
- While reading the .janno file trident trims all leading and trailing whitespaces around individual cells. Also
- 94 all instances of the No-Break Space unicode character will be removed. This means these whitespaces will not
- be preserved when a package is forged.

3 Package creation and manipulation commands

$_{97}$ 3.1 Init command

- init creates a new Poseidon package from genotype data files. It adds a POSEIDON.yml file, a dummy .janno file for context information and an empty .bib file for literature references.
- 100 Command line details

```
Usage: trident init ((-p|--genoOne FILE) | --inFormat FORMAT --genoFile FILE
--snpFile FILE --indFile FILE) [--snpSet SET]
(-o|--outPackagePath DIR) [-n|--outPackageName STRING]
[--minimal]
```

Create a new Poseidon package from genotype data

Available options:

л	variable options.	
	-h,help	Show this help text
	-p,genoOne FILE	One of the input genotype data files. Expects .bed,
		.bim or .fam for PLINK and .geno, .snp or .ind for
		EIGENSTRAT. The other files must be in the same
		directory and must have the same base name.
	inFormat FORMAT	The format of the input genotype data: EIGENSTRAT or
		PLINK. Only necessary for data input withgenoFile
		+snpFile +indFile.
	genoFile FILE	Path to the input geno file.
	snpFile FILE	Path to the input snp file.
	indFile FILE	Path to the input ind file.
	snpSet SET	The snpSet of the package: 1240K, HumanOrigins or
		Other. Only relevant for data input with -p genoOne

```
or --genoFile + --snpFile + --indFile, because the
packages in a -d|--baseDir already have this
information in their respective POSEIDON.yml files.
(default: Other)

-o,--outPackagePath DIR Path to the output package directory.
-n,--outPackageName STRING

The output package name. This is optional: If no name
is provided, then the package name defaults to the
basename of the (mandatory) --outPackagePath
argument. (default: Nothing)

--minimal Should the output data be reduced to a necessary
minimum and omit empty scaffolding?
```

101 The command

```
trident init \
    --inFormat EIGENSTRAT/PLINK \
    --genoFile path/to/genoFile \
    --snpFile path/to/snpFile \
    --indFile path/to/indFile \
    --snpSet 1240K|HumanOrigins|Other \
    -o path/to/new_package_name
```

requires the format (--inFormat) of your input data (either EIGENSTRAT or PLINK), the paths to the respective files (--genoFile, --snpFile, --indFile), and optionally the "shape" of these files (--snpSet), so if they cover the 1240K, the HumanOrigins or an Other SNP set.

A simpler interface is available with -p (+ --snpSet), which only requires a path to one of the genotype data files and automatically discovers the others if they share the same base name:

```
trident init \
  -p path/to/genoFile \
  --snpSet 1240K|HumanOrigins|Other \
  -o path/to/new_package_name
```

The following file extensions are expected:

	EIGENSTRAT	PLINK
genoFile	.geno	.bed
${\rm snpFile}$.snp	.bim
$\operatorname{indFile}$.ind	.fam

The output package created by init is located in a new directory -o, which should not already exist when init is called, and gets the package title corresponding to the basename of -o. You can also set the title explicitly with -n.

The --minimal flag causes init to create a minimal package with a very basic POSEIDON.yml and no .bib and .janno files.

3.2 Fetch command

fetch allows to download Poseidon packages from a remote Poseidon server via a Web API. This server provides
 all packages in the Poseidon public archives.

16 Command line details

```
Usage: trident fetch (-d|--baseDir DIR)
                     (--downloadAll |
                       (--fetchFile FILE | (-f|--fetchString DSL)))
                     [--remoteURL URL] [--archive STRING]
  Download data from a remote Poseidon repository
Available options:
  -h,--help
                           Show this help text
  -d,--baseDir DIR
                           A base directory to search for Poseidon packages.
  --downloadAll
                           Download all packages the server is offering.
  --fetchFile FILE
                           A file with a list of packages. Works just as -f, but
                           multiple values can also be separated by newline, not
                           just by comma. -f and --fetchFile can be combined.
  -f,--fetchString DSL
                           List of packages to be downloaded from the remote
                           server. Package names should be wrapped in asterisks:
                           *package_title*. You can combine multiple values with
                           comma, so for example: "*package_1*, *package_2*,
                           *package_3*". fetchString uses the same parser as
                           forgeString, but does not allow excludes. If groups
                           or individuals are specified, then packages which
                           include these groups or individuals are included in
                           the download.
                           URL of the remote Poseidon server.
  --remoteURI, URI,
                           (default: "https://server.poseidon-adna.org")
  --archive STRING
                           The name of the Poseidon package archive that should
                           be queried. If not given, then the query falls back
                           to the default archive of the server selected with
                           --remoteURL. See the archive documentation at
                           https://www.poseidon-adna.org/#/archive_overview for
                           a list of archives currently available from the
                           official Poseidon Web API. (default: Nothing)
```

117 It works with

```
trident fetch -d ... -d ... \
  -f "*package_title_1*,*package_title_2-1.0.1*,group_name,<individual1>"
```

and the entities you want to download must be listed either in a simple string of comma-separated values, which can be passed via -f/--fetchString, or in a text file (--fetchFile). Entities are then combined from these sources.

Entities are specified using a special syntax (see also the documentation of forge below): packages are wrapped in asterisks, with or without a version number appended after a dash (e.g. *package_title* or *package_title-1.2.3), group names are spelled as is, and individual names are wrapped in angular brackets (e.g. <individual1>). Fetch will figure out which packages need to be downloaded to include all specified entities.

--downloadAll, which can be given instead of -f and --fetchFile, causes fetch to download all packages from

--downloadAll, which can be given instead of -f and --fetchFile, causes fetch to download all packages from the server. The downloaded packages are added in the first (!) -d directory (which gets created if it doesn't exist), but downloads are only performed if the respective packages are not already present in the latest version in any of the -d directories.

Note that trident fetch is usually used in a workflow with trident list --remote: First one inspects what is available on the server with list, to then compile a custom, targeted fetch command.

fetch has the optional arguments --remote https:://..." to name an alternative Poseidon server and --archive to select a specific Poseidon archive on the server.

3.3 Forge command

forge creates new Poseidon packages by extracting and merging packages, populations and individuals/samples from Poseidon repositories.

136 Command line details

```
Usage: trident forge ((-d|--baseDir DIR) |

((-p|--genoOne FILE) | --inFormat FORMAT --genoFile FILE

--snpFile FILE --indFile FILE) [--snpSet SET])

[--forgeFile FILE | (-f|--forgeString DSL)]

[--selectSnps FILE] [--intersect] [--outFormat FORMAT]

[--minimal] [--onlyGeno] (-o|--outPackagePath DIR)

[-n|--outPackageName STRING] [--packagewise]

[--outPlinkPopName MODE]
```

Select packages, groups or individuals and create a new Poseidon package from them

Available options:

ivaliable options.	
-h,help	Show this help text
-d,baseDir DIR	A base directory to search for Poseidon packages.
-p,genoOne FILE	One of the input genotype data files. Expects .bed,
	.bim or .fam for PLINK and .geno, .snp or .ind for
	EIGENSTRAT. The other files must be in the same
	directory and must have the same base name.
inFormat FORMAT	The format of the input genotype data: EIGENSTRAT or
	PLINK. Only necessary for data input withgenoFile
	+snpFile +indFile.
genoFile FILE	Path to the input geno file.
snpFile FILE	Path to the input snp file.
indFile FILE	Path to the input ind file.
snpSet SET	The snpSet of the package: 1240K, HumanOrigins or

Other. Only relevant for data input with -p|--genoOne or --genoFile + --snpFile + --indFile, because the packages in a -d|--baseDir already have this information in their respective POSEIDON.yml files. (default: Other)

--forgeFile FILE

A file with a list of packages, groups or individual samples. Works just as -f, but multiple values can also be separated by newline, not just by comma. Empty lines are ignored and comments start with "#", so everything after "#" is ignored in one line. Multiple instances of -f and --forgeFile can be given. They will be evaluated according to their input order on the command line.

-f,--forgeString DSL

List of packages, groups or individual samples to be combined in the output package. Packages follow the syntax *package_title*, populations/groups are simply group_id and individuals <individual_id>. You can combine multiple values with comma, so for example: "*package_1*, <individual_1>, <individual_2>, group_1". Duplicates are treated as one entry. Negative selection is possible by prepending "-" to the entity you want to exclude (e.g. "*package 1*, -<individual_1>, -group_1"). forge will apply excludes and includes in order. If the first entity is negative, then forge will assume you want to merge all individuals in the packages found in the baseDirs (except the ones explicitly excluded) before the exclude entities are applied. An empty forgeString (and no --forgeFile) will therefore merge all available individuals. If there are individuals in your input packages with equal individual id, but different main group or source package, they can be specified with the special syntax "<package:group:individual>".

--selectSnps FILE

To extract specific SNPs during this forge operation, provide a Snp file. Can be either Eigenstrat (file ending must be '.snp') or Plink (file ending must be '.bim'). When this option is set, the output package will have exactly the SNPs listed in this file. Any SNP not listed in the file will be excluded. If option '--intersect' is also set, only the SNPs overlapping between the SNP file and the forged packages are output. (default: Nothing)
Whether to output the intersection of the genotype files to be forged. The default (if this option is

--intersect

not set) is to output the union of all SNPs, with genotypes defined as missing in those packages which do not have a SNP that is present in another package. With this option set, the forged dataset will typically have fewer SNPs, but less missingness. The format of the output genotype data: EIGENSTRAT or --outFormat FORMAT PLINK. (default: PLINK) --minimal Should the output data be reduced to a necessary minimum and omit empty scaffolding? --onlyGeno Should only the resulting genotype data be returned? This means the output will not be a Poseidon package. -o,--outPackagePath DIR Path to the output package directory. -n, -- outPackageName STRING The output package name. This is optional: If no name is provided, then the package name defaults to the basename of the (mandatory) --outPackagePath argument. (default: Nothing) Skip the within-package selection step in forge. This --packagewise will result in outputting all individuals in the relevant packages, and hence a superset of the requested individuals/groups. It may result in better performance in cases where one wants to forge entire packages or almost entire packages. Details: Forge conceptually performs two types of selection: First, it identifies which packages in the supplied base directories are relevant to the requested forge, i.e. whether they are either explicitly listed using *PackageName*, or because they contain selected individuals or groups. Second, within each relevant package, individuals which are not requested are removed. This option skips only the second step, but still performs the first. --outPlinkPopName MODE Where to write the population/group name into the FAM file in Plink-format. Three options are possible: asFamily (default) | asPhenotype | asBoth. See also

forge can be used with

```
trident forge -d ... -d ... \
  -f "*package_name*, group_id, <individual_id>" \
  -o path/to/new_package_name
```

--inPlinkPopName.

where the entities (packages, groups/populations, individuals/samples) you want in the output package can be
denoted either as a string on the command line (-f/--forgeString), or in an input text file (--forgeFile).

See the section below for the syntax of this selection language. Do not forget to wrap the --forgeString query

in quotes.

154

155

156

157

158

159

160

161

162

163

165

Including one or multiple Poseidon packages with -d is not the only way to include data for a forge operation.

It is also possible to consider unpackaged genotype data directly with -p (+ --snpSet) or --inFormat +
--genoFile + --snpFile + --indFile (+ --snpSet). This makes the following example possible, where we
merge data from one Poseidon package and two unpackaged genotype datasets to get a new EIGENSTRAT
dataset.

```
trident forge \
  -d 2017_GonzalesFortesCurrentBiology \
  -p 2018_VeeramahPNAS/2018_VeeramahPNAS.fam \
  --inFormat PLINK \
  --genoFile 2017_HaberAJHG/2017_HaberAJHG.bed \
  --snpFile 2017_HaberAJHG/2017_HaberAJHG.bim \
  --indFile 2017_HaberAJHG/2017_HaberAJHG.fam \
  -f "<STR241.SG>,<ERS1790729.SG>,Iberia_HG.SG" \
  -o testpackage \
  --outFormat EIGENSTRAT \
  --onlyGeno
```

3.3.1 The forge selection language

The text in --forgeString and --forgeFile (and with a reduced syntax also in --fetchString and --fetchFile) are parsed as a domain specific query language that describes precisely which entities should be compiled in the output package of a given forge operation. The language has multiple syntactic elements and a specific evaluation logic.

In general a --forgeString query consists of multiple entities, separated by ,. The main entities are Poseidon packages, groups/populations and individuals/samples:

- Each package title is surrounded by *: *package*. That means if you want all individuals of the Poseidon
 package 2019_Jeong_InnerEurasia in the output package you would add *2019_Jeong_InnerEurasia*
 to the query.
- Groups/populations are not specially marked: group. So to get all individuals of the group Swiss_Roman_Period, you would simply add Swiss_Roman_Period.
- Individuals/samples are surrounded by < and >: <individual>. ALA026 therefore becomes <ALA026>. A second way to denote individuals is with the more verbose and specific syntax <package:group:individual>. Such defined individuals take precedence over differently defined ones (so directly with <individual> or as a subset of *package* or group). This allows to resolve duplication issues precisely at least in cases where the duplicated individuals differ in source package or primary group.
- Package versions can be appended to package names, such as *package-1.2.3*.
- This also works with the verbose individual syntax: <package-1.2.3:group:individual>.

In the --forgeFile each line is treated as a separate forgeString, empty lines are ignored and # symbols start comments. So this is a valid example of a forgeFile:

```
# Packages
*pac1*, *pac2-1.2.3*
```

By prepending - to entities, we can exclude them from the forged package (this feature is not available for fetch). forge figures out the final list of samples to include by interpreting all forge-entities in order. So an entity list *pac1*,-<ind1>,group1 may result in a different outcome than *pac1*,group1,-<ind1>, depending on whether <ind1> belongs to group1 or not.

172 If the forge entity list starts with a negative entity, or if the entity list is empty, forge will implicitly assume 173 you want to include all individuals in all **latest** versions of packages found in the base directories (except the 174 ones explicitly excluded, of course).

175 The specific semantics of the various ways to include or exclude entities are as follows:

176 3.3.1.1 Inclusion queries

177

179

180

186

187

189

190

191

192

193

199

200

- *pac1*: Select all individuals in the latest version of package "pac1"
- *pac1-1.0.1*: Select all individuals in package "pac1" with version "1.0.1"
 - group1: Select all individuals associated with "group1" in all latest versions of all packages
 - <ind1>: Select the individual named "ind1", searching in all latest packages.
- <pac1:group1:ind1>: Select the individual named "ind1" associated with "group1" in the latest version of package "pac1"
- <pac1-1.0.1:group1:ind1>: Select the individual named "ind1" associated with "group1" in the package "pac1" with version "1.0.1"

185 3.3.1.2 Exclusion queries

- -*pac1*: Remove all individuals in all versions of package "pac1"
- -*pac1-1.0.1*: Remove only individuals in package "pac1" with version "1.0.1" (but leave other versions in)
- -group1: Remove all individuals associated with "group1" in all versions of all packages (not just the latest)
 - -<ind1>: Remove all individuals named "ind1" in all versions of all packages (not just the latest)
- -<pac1:group1:ind1>: Remove the individual named "ind1" associated with "group1", searching in all versions of package "pac1"
- -<pac1-1.0.1:group1:ind1>: Remove the individual named "ind1" associated with "group1", but only if they are in "pac1" with version "1.0.1"

196 If a query results in multiple individuals with the same name, forge will throw an error.

197 3.3.2 Treatment of the genotype data while merging

Forge performs a series of steps to merge the genotype data of multiple source files:

1. Genotype data from each package is streamed in parallel. Because our packages may have different SNP locations (specified by chromosome-position pairs) listed in their .bim/.snp file, we first perform a zipping-

operation, whose behaviour depends on whether --intersect is set or not. Without --intersect, any SNP position listed in any package will be forwarded to the output, with missing values being filled in in all packages that do not list that particular SNP. With --intersect, only SNP positions that are present in all packages are considered. Note that relevant for this step is only whether a given SNP position is part of the genotype data, not whether the actual genotypes are missing or not.

- 2. At each SNP, the consensus alleles are selected, by collecting all reference and alternative alleles from all sources. If more than two non-dummy alleles (alleles different from N) are present in that collection, an error is thrown. If exactly two non-dummy alleles are present (which should be the case for binary SNPs), the two alleles are declared "reference" and "alternative" alleles for the output. If only one non-dummy allele is present, it is set to be the reference allele, and "N" is set to be the alternative.
- 3. All source genotype data is then read and recoded in terms of the two chosen consensus alleles. This will make sure that source data with flipped reference and alternative allele gets correctly merged in.
- 4. SNP IDs, as part of PLINK .bim files are checked across the source files. If all SNP IDs for a given SNP are missing, then the result will also be missing. If there is only one SNP ID present in some or all source packages, that ID gets forwarded to the output. In the (unusual) case that there are multiple different non-missing SNP IDs (of the form "rs" followed by a number), then a debug warning is output (which gets printed to the screen when --debug is selected), and simply the first value is chosen to be output into the forged .bim file. We decided not to throw an error in that case, because we consider the physical position of the SNP (specified by Chromosome and position) to be definitive, and the SNP ID to be of secondary importance.
- 5. Genetic positions, as part of PLINK .bim files are checked in a similar manner, with "0.0" being interpreted as missing.

3.3.3 Treatment of the .janno file while merging

forge merges and subsets .janno files along with the genotype data. If a package lacks a .janno file, then a basic one will be created internally an on-the-fly based on the information in the genotype data, and used for the output. Missing columns across packages will be filled with n/a.

For merging two .janno files $\bf A$ and $\bf B$ the following rules apply regarding undefined, arbitrary additional columns:

- If A has an additional column which is not in B then empty cells in the rows imported from B are filled with n/a.
- If A and B share additional columns with identical column name, then they are treated as semantically identical units and merged accordingly.
- In the resulting .janno file, all additional columns from both A and B are sorted alphabetically and appended after the normal, specified variables.

235 The following example illustrates the described behaviour:

236 A.janno

Poseidon_ID	${\bf Group_Name}$	${\rm Genetic_Sex}$	AdditionalColumn1	AdditionalColumn2
XXX011	POP1	M	A	D
XXX012	POP2	F	В	E
XXX013	POP1	M	C	F

237 B.janno

Poseidon_ID	Group_Name	Genetic_Sex	AdditionalColumn3	AdditionalColumn2
YYY022	POP5	F	G	J
YYY023	POP5	F	Н	K
YYY024	POP5	M	I	L

A.janno + B.janno

Poseidon_ID	Group_Name	e Genetic_Sex	AdditionalColumn1	AdditionalColumn2	AdditionalColumn3
XXX011	POP1	M	A	D	n/a
XXX012	POP2	F	В	\mathbf{E}	n/a
XXX013	POP1	M	\mathbf{C}	F	n/a
YYY022	POP5	F	n/a	J	G
YYY023	POP5	F	n/a	K	H
YYY024	POP5	M	n/a	L	I

3.3.4 Treatment of the .ssf file while merging

The Sequencing Source File (short .ssf file) is forged in exactly the same way as the .janno file. .ssf files
that are present are included in the forge product, following selection of those entities which are listed in the
poseidon_IDs columns. Columns that are only present in some packages, including those not defined in the
Poseidon package specification, are also included in the forged product in the same way as described for .janno
files above.

245 3.3.5 Treatment of the .bib file while merging

In the forge process all relevant samples for the output package are determined. This includes their .janno entries and therefore the information on the publication keys documented for them in the .janno Publication column. The output .bib file compiles only the relevant references for the samples in the output package. It includes the references exactly once and is sorted alphabetically by key.

$_{250}$ 3.3.6 Other options

- Just as for init the output package of forge is created as a new directory -o. The title can also be explicitly defined with -n.
- --minimal allows for the creation of a minimal output package without .bib and .janno. This is especially useful for data analysis pipelines, where only the genotype data is required. Even more basic output comes with --onlyGeno, which means that only the genotype data is returned without any Poseidon package.
- forge has a an optional flag --intersect, that defines, if the genotype data from different packages should be merged with a union or an intersect operation. See *Treatment of the genotype data while merging* above.
- 258 --intersect also influences the automatic determination of the snpSet field in the POSEIDON.yml file for the
 259 resulting package. If the snpSets of all input packages are identical, then the resulting package will just inherit
 260 this configuration. Otherwise forge applies the following pairwise merging logic:

Input snpSet A	Input snpSet B	intersect	Ouput snpSet
Other	*	*	Other
$1240 \mathrm{K}$	HumanOrigins	True	HumanOrigins
$1240 \mathrm{K}$	HumanOrigins	False	1240K

--selectSnps allows to provide forge with a SNP file in EIGENSTRAT (.snp) or PLINK (.bim) format to 261 create a package with a specific selection. When this option is set, the output package will have exactly the 262 SNPs listed in this file. Any SNP not listed in the file will be excluded. If --intersect is also set, only the 263 SNPs overlapping between the SNP file and the forged packages are output. 264

With --packagewise the within-package selection step in forge can be skipped. This will result in outputting all individuals in the relevant packages, and hence a superset of the requested individuals/groups. It may result 266 in better performance in cases where one wants to forge entire packages. 267

Genoconvert command

genoconvert converts the genotype data in a Poseidon package to a different file format. The respective entries 269 in the POSEIDON.yml file are changed accordingly. 270

Command line details

```
Usage: trident genoconvert ((-d|--baseDir DIR) |
                             ((-p|--genoOne FILE) | --inFormat FORMAT
                               --genoFile FILE --snpFile FILE --indFile FILE)
                             [--snpSet SET]) --outFormat FORMAT [--onlyGeno]
                            [-o|--outPackagePath DIR] [--removeOld]
                            [--outPlinkPopName MODE] [--onlyLatest]
  Convert the genotype data in a Poseidon package to a different file format
Available options:
  -h,--help
                           Show this help text
  -d,--baseDir DIR
                           A base directory to search for Poseidon packages.
```

-p,--genoOne FILE One of the input genotype data files. Expects .bed, .bim or .fam for PLINK and .geno, .snp or .ind for EIGENSTRAT. The other files must be in the same directory and must have the same base name. --inFormat FORMAT The format of the input genotype data: EIGENSTRAT or PLINK. Only necessary for data input with --genoFile + --snpFile + --indFile. --genoFile FILE Path to the input geno file. --snpFile FILE Path to the input snp file. --indFile FILE Path to the input ind file. The snpSet of the package: 1240K, HumanOrigins or --snpSet SET Other. Only relevant for data input with -p|--genoOne or --genoFile + --snpFile + --indFile, because the

```
packages in a -d|--baseDir already have this
                         information in their respective POSEIDON.yml files.
                         (default: Other)
--outFormat FORMAT
                         the format of the output genotype data: EIGENSTRAT or
                         PLINK.
                         Should only the resulting genotype data be returned?
--onlyGeno
                         This means the output will not be a Poseidon package.
-o,--outPackagePath DIR
                         Path to the output package directory. This is
                         optional: If no path is provided, then the output is
                         written to the directories where the input genotype
                         data file (.bed/.geno) is stored. (default: Nothing)
                         Remove the old genotype files when creating the new
--removeOld
                         ones.
--outPlinkPopName MODE
                         Where to write the population/group name into the FAM
                         file in Plink-format. Three options are possible:
                         asFamily (default) | asPhenotype | asBoth. See also
                         --inPlinkPopName.
--onlyLatest
                         Consider only the latest versions of packages, or the
                         groups and individuals within the latest versions of
                         packages, respectively.
```

272 With the default setting

```
trident genoconvert -d ... -d ... --outFormat EIGENSTRAT|PLINK
```

273 all packages in -d will be converted to the desired --outFormat (either EIGENSTRAT or PLINK), if the data is 274 not already in this format. This includes updating the respective POSEIDON.yml files.

The "old" data is not deleted, but kept around. That means conversion can result in a package with both PLINK and EIGENSTRAT data, but only one is linked in the POSEIDON.yml file, and that is what will be used by trident. To delete the old data in the conversion you can add the --removeOld flag.

²⁷⁸ -p (+ --snpSet) or --inFormat + --genoFile + --snpFile + --indFile (+ --snpSet) allow to directly convert genotype data that is not wrapped in a Poseidon package and store it to a directory given in -o. See this example:

```
trident genoconvert \
  -p 2018_Mittnik_Baltic/Mittnik_Baltic.bed \
  --outFormat EIGENSTRAT \
  -o my_directory
```

281 3.5 Jannocoalesce command

jannocoalesce merges information from one or multiple source .janno files into a target .janno file.

283 Command line details

```
Usage: trident jannocoalesce ((-s|--sourceFile FILE) | (-d|--baseDir DIR))

(-t|--targetFile FILE) [-o|--outFile FILE]

[--includeColumns ARG | --excludeColumns ARG]
```

```
[-f|--force] [--sourceKey ARG] [--targetKey ARG]
                           [--stripIdRegex ARG]
Coalesce information from one or multiple janno files to another one
```

Available options:

-h,help	Show this help text
-s,sourceFile FILE	The source .janno file.
-d,baseDir DIR	A base directory to search for Poseidon packages.
-t,targetFile FILE	The target .janno file to fill.
-o,outFile FILE	An optional file to write the results to. If not
	specified change the target file in place

If not specified, change the target file in place.

(default: Nothing)

--includeColumns ARG A comma-separated list of .janno column names to coalesce. If not specified, all columns that can be found in the source and target will get filled. --excludeColumns ARG A comma-separated list of .janno column names NOT to

coalesce. All columns that can be found in the source and target will get filled, except the ones listed

here.

-f,--force With this option, potential non-missing content in target columns gets overridden with non-missing content in source columns. By default, only missing

data gets filled-in.

--sourceKey ARG The .janno column to use as the source key.

(default: "Poseidon_ID")

--targetKey ARG The .janno column to use as the target key.

(default: "Poseidon_ID")

--stripIdRegex ARG An optional regular expression to identify parts of

> the IDs to strip before matching between source and target. Uses POSIX Extended regular expressions.

A most basic run may just include two arguments:

```
trident jannocoalesce \
  --sourceFile path/to/source.janno \
  --targetFile path/to/target.janno
```

jannocoalesce generally works by reading a source .janno file with -s|--sourceFile (or all .janno files in a 285 -d|--baseDir) and a target .janno file with -t|--targetFile. 286

It then merges these files by a key column, which can be selected with --sourceKey and --targetKey. The default for both of these key columns is the Poseidon_ID. In case the entries in the key columns slightly and 288 systematically differ, e.g. because the Poseidon_IDs in either have a special suffix (for example _SG), then the 289 --stripIdRegex option allows to strip these with a regular expression to thus match the keys.

jannocoalesce generally attempts to fill all empty cells in the target . janno file with information from the

source. --includeColumns and --excludeColumns allow to select specific columns for which this should be
done. In some cases it may be desirable to not just fill empty fields in the target, but overwrite the information
already there with the -f|--force option. If the target file should be preserved, then the output can be directed
to a new output .janno file with -o|--outFile.

96 3.6 Rectify command

rectify automatically harmonizes POSEIDON.yml files of one or multiple packages. This is not an automatic update from one Poseidon version to the next, but rather a clean-up wizard after manual modifications.

299 Command line details

```
Usage: trident rectify (-d|--baseDir DIR) [--ignorePoseidonVersion]
                       [--poseidonVersion ?.?.?]
                       [--packageVersion VPART [--logText STRING]]
                       [--checksumAll | [--checksumGeno] [--checksumJanno]
                         [--checksumSSF] [--checksumBib]]
                       [--newContributors DSL] [--onlyLatest]
  Adjust POSEIDON.yml files automatically to package changes
Available options:
  -h,--help
                           Show this help text
  -d,--baseDir DIR
                           A base directory to search for Poseidon packages.
  --ignorePoseidonVersion Read packages even if their poseidonVersion is not
                           compatible with trident.
  --poseidonVersion ?.?.?
                           Poseidon version the packages should be updated to:
                           e.g. "2.5.3".
  --packageVersion VPART
                           Part of the package version number in the
                           POSEIDON.yml file that should be updated: Major,
                           Minor or Patch (see https://semver.org).
                           Log text for this version in the CHANGELOG file.
  --logText STRING
  --checksumAll
                           Update all checksums.
  --checksumGeno
                           Update genotype data checksums.
  --checksumJanno
                           Update .janno file checksum.
  --checksumSSF
                           Update .ssf file checksum
  --checksumBib
                           Update .bib file checksum.
  --newContributors DSL
                           Contributors to add to the POSEIDON.yml file in the
                           form "[Firstname Lastname] (Email address);...".
                           Consider only the latest versions of packages, or the
  --onlyLatest
                           groups and individuals within the latest versions of
                           packages, respectively.
```

It can be called with a lot of optional arguments. Note that rectify by default does **not** apply any changes if none of these arguments are set. Each change requires explicit opt-in.

```
trident rectify -d ... -d ... \
   --poseidonVersion "X.X.X" \
```

```
--packageVersion Major|Minor|Patch \
--logText "short description of the update" \
--checksumAll \
--newContributors "[Firstname Lastname] (Email address);..."
```

302 The following arguments determine which fields of the POSEIDON.yml file should be modified:

- --poseidonVersion allows a simple change of the poseidonVersion field in the POSEIDON.yml file.
- --packageVersion increments the package version number in the first, the second or the third position.
 It can optionally be called with --logText, which appends an entry to the CHANGELOG file for the respective package version update. --logText also creates a new CHANGELOG.md file if it does not exist yet.
- --checksumGeno, --checksumJanno, --checksumSSF and --checksumBib add or modify the respective checksum fields in the POSEIDON.yml file. --checksumAll is a wrapper to call all of them at once.
- --newContributors adds new contributors.

As rectify reads and rewrites POSEIDON.yml files, it may change their inner order, layout or even content (e.g. if
they have fields which are not in the POSEIDON.yml specification). Create a backup of the POSEIDON.yml file
before running rectify if you are uncertain if this might affect you negatively.

314 4 Inspection commands

4.1 List command

list lists packages, groups and individuals of local datasets, or of packages available in the archives on the web server.

Command line details

304

305

307

309

310

315

```
Usage: trident list ((-d|--baseDir DIR) | --remote [--remoteURL URL]
                      [--archive STRING])
                    (--packages | --groups | --individuals
                      [-j|--jannoColumn COLNAME]) [--raw] [--onlyLatest]
  List packages, groups or individuals from local or remote Poseidon
  repositories
Available options:
  -h,--help
                           Show this help text
                           A base directory to search for Poseidon packages.
  -d,--baseDir DIR
                           List packages from a remote server instead the local
  --remote
                           file system.
  --remoteURL URL
                           URL of the remote Poseidon server.
                            (default: "https://server.poseidon-adna.org")
  --archive STRING
                           The name of the Poseidon package archive that should
                           be queried. If not given, then the query falls back
                           to the default archive of the server selected with
                            --remoteURL. See the archive documentation at
```

```
https://www.poseidon-adna.org/#/archive_overview for
                         a list of archives currently available from the
                         official Poseidon Web API. (default: Nothing)
                         List all packages.
--packages
                         List all groups, ignoring any group names after the
--groups
                         first as specified in the .janno-file.
--individuals
                         List all individuals/samples.
-j,--jannoColumn COLNAME List additional fields from the janno files, using
                         the .janno column heading name, such as "Country",
                         "Site", "Date_C14_Uncal_BP", etc..
                         Return the output table as tab-separated values
--raw
                         without header. This is useful for piping into grep
                         or awk.
--onlyLatest
                         Consider only the latest versions of packages, or the
                         groups and individuals within the latest versions of
                         packages, respectively.
```

To list packages from your local repositories, as seen above you can run

```
trident list -d ... -d ... --packages
```

- This will yield a nicely formatted table of all packages, their version and the number of individuals in them.
- You can use --remote to show packages on the remote server. For example

```
trident list --packages --remote --archive "community-archive"
```

- will result in a view of all packages available in one of the public Poseidon archives. Just as for fetch, the
 --archive flag allows to choose which public archive to query.
- Independent of whether you query a local or an online archive, you can not just list packages, but also groups, as defined in the third column of EIGENSTRAT .ind files (or the first/last column of a PLINK .fam file), and individuals with the flags --groups and --individuals (instead of --packages).
- The --individuals flag additionally provides a way to immediately access information from .janno files on the command line. This works with the -j|--jannoColumn option. For example adding -j Country -j

 Date_C14_Uncal_BP to the commands above will add the Country and the Date_C14_Uncal_BP columns to the respective output tables.
- Note that if you want a less ornate table, for example because you want to load this into Excel, or pipe into another command that cannot deal with the table layout, you can use the --raw option to output that table as a simple tab-delimited stream.

334 4.2 Summarise command

- summarise prints some general summary statistics for a given Poseidon dataset taken from the .janno files.
- 336 Command line details

```
Usage: trident summarise (-d|--baseDir DIR) [--raw]
```

Get an overview over the content of one or multiple Poseidon packages

Available options:

-h,--help Show this help text

-d,--baseDir DIR A base directory to search for Poseidon packages.
--raw Return the output table as tab-separated values

without header. This is useful for piping into grep

or awk.

You can run it with

trident summarise -d ... -d ...

- which will show you context information like among others the number of individuals in the dataset, their sex
- distribution, the mean age of the samples or the mean coverage on the 1240K SNP array in a table. summarise
- $_{340}$ depends on complete . janno files and will silently ignore missing information.
- You can use the --raw option to output the summary table in a simple, tab-delimited layout.

$_{\scriptscriptstyle 2}$ 4.3 Survey command

- survey tries to indicate package completeness (mostly focused on .janno files) for Poseidon datasets.
- 344 Command line details

Usage: trident survey (-d|--baseDir DIR) [--raw] [--onlyLatest]

Survey the degree of context information completeness for Poseidon packages

Available options:

-h,--help Show this help text

-d,--baseDir DIR A base directory to search for Poseidon packages.
--raw Return the output table as tab-separated values

without header. This is useful for piping into grep

or awk.

--onlyLatest Consider only the latest versions of packages, or the

groups and individuals within the latest versions of

packages, respectively.

345 Running

trident survey -d ... -d ...

- $_{346}$ will yield a table with one row for each package. See trident survey -h for a legend which cell of this table
- means what.
- 348 Again you can use the --raw option to output the survey table in a tab-delimited format.

349 4.4 Validate command

validate checks Poseidon packages and individual package components for structural correctness.

351 Command line details

Usage: trident validate ((-d|--baseDir DIR) [--ignoreGeno] [--fullGeno] [--ignoreDuplicates] [-c|--ignoreChecksums] [--ignorePoseidonVersion] | --pyml FILE | (-p|--genoOne FILE) | --inFormat FORMAT --genoFile FILE --snpFile FILE --indFile FILE | --janno FILE | --ssf FILE | --bib FILE) [--noExitCode] [--onlyLatest] Check Poseidon packages or package components for structural correctness Available options: -h,--help Show this help text -d,--baseDir DIR A base directory to search for Poseidon packages. --ignoreGeno Ignore snp and geno file. Test parsing of all SNPs (by default only the first --fullGeno 100 SNPs are probed). Do not stop on duplicated individual names in the --ignoreDuplicates package collection. -c,--ignoreChecksums Whether to ignore checksums. Useful for speedup in debugging. --ignorePoseidonVersion Read packages even if their poseidonVersion is not compatible with trident. --pyml FILE Path to a POSEIDON.yml file. -p,--genoOne FILE One of the input genotype data files. Expects .bed, .bim or .fam for PLINK and .geno, .snp or .ind for EIGENSTRAT. The other files must be in the same directory and must have the same base name. --inFormat FORMAT The format of the input genotype data: EIGENSTRAT or PLINK. Only necessary for data input with --genoFile + --snpFile + --indFile. Path to the input geno file. --genoFile FILE --snpFile FILE Path to the input snp file. --indFile FILE Path to the input ind file. Path to a .janno file. --janno FILE --ssf FILE Path to a .ssf file. Path to a .bib file. --bib FILE --noExitCode Do not produce an explicit exit code. --onlyLatest Consider only the latest versions of packages, or the

You can run it with

packages, respectively.

groups and individuals within the latest versions of

trident validate -d ... -d ...

361

363

364

366

367

369

to check packages and it will either report a success (Validation passed) or failure with specific error messages.

Instead of validating entire packages with -d you can also apply it to individual files and package components: --pyml (POSEIDON.yml), -p | --inFormat + --genoFile + --snpFile + --indFile (genotype
data), --janno (.janno file), --ssf (.ssf file) or --bib (.bib file). In this case validate attempts to read and
parse the respective files individually and reports any issues it encounters. Note that this considers the files in
isolation and does not include any cross-file consistency checks.

When applied to packages, validate tries to ensure that each package adheres to the Poseidon package specification. Here is a list of what is checked:

- Structural correctness of the POSEIDON.yml file.
- Presence of all files references in the POSEIDON.yml file.
 - Full structural correctness of .janno, .ssf and .bib file.
- Superficial correctness of genotype data files by parsing the first 100 SNPs. A full check that parses all SNPs can be triggered with the --fullGeno option. --ignoreGeno, on the other hand, causes validate to ignore the genotype data entirely, which speeds up the validation significantly.
 - Correspondence of BibTeX keys in .bib and .janno
 - Correspondence of sample IDs in .janno and .ssf.
 - Correspondence of sample and group IDs in . janno and genotype data files.

In fact much of this validation already runs as part of the general package reading pipeline invoked for other trident subcommands (e.g. forge). validate is meant to be more thorough and brittle, though, and will explicitly fail if even a single package is broken. For special cases more flexibility can be enabled with the options

--ignoreDuplicates, --ignoreChecksums and --ignorePoseidonVersion.

Remember to run validate with --debug to get more information in case the default output is not sufficient to analyse an issue.