

## Data Assembly

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This script assembles simulated phase 1 data.

Make sure you are in the script directory, where this files resides.

Listing 1:

```
> getwd()

[1] "/data/metrumrg/inst/example/project/script"
```

Load the metrumrg package.

Listing 2:

```
> library(metrumrg)
```

Groom the dose data

Listing 3:

```
> dose <- read.csv('../data/source/dose.csv', na.strings='.', stringsAsFactors=FALSE)
> head(dose)
```

	SUBJ	AMT	HOURL
1	1	1e+03	0
2	2	5e+03	0
3	3	1e+04	0
4	4	5e+04	0
5	5	1e+05	0
6	6	1e+03	0

Listing 4:

```
> dose <- as.keyed(dose, key=c('SUBJ', 'HOURL'))
> summary(dose)
```

```
SUBJ~HOURL
0 NA keys
0 duplicate keys
```

Looks okay.

Groom the demographic data.

Listing 5:

```
> dem <- read.csv('../data/source/dem.csv', na.strings='.', stringsAsFactors=FALSE)
> head(dem)
```

	SUBJ	HEIGHT	WEIGHT	SEX	AGE	DOSE	FED	SMK	DS	CRCN
1	1	174	74.2	0	29.1	1e+03	1	0	0	83.5
2	2	177	80.3	0	36.8	5e+03	1	0	0	142.0
3	3	180	94.2	0	46.4	1e+04	1	0	0	121.0
4	4	177	85.2	0	30.3	5e+04	1	0	0	127.0
5	5	166	82.8	0	32.5	1e+05	1	0	0	97.2
6	6	164	63.9	0	18.8	1e+03	1	0	0	138.0

Listing 6:

```
> dem <- as.keyed(dem, key='SUBJ')
> summary(dem)
```

```
SUBJ
0 NA keys
0 duplicate keys
```

Looks okay. Note that DOSE is a treatment group, not an actual dose.

Groom the pk data.

Listing 7:

```
> pk <- read.csv('../data/source/pk.csv', na.strings='.', stringsAsFactors=FALSE)
> head(pk)
```

```
  SUBJ HOUR    DV
1     1  0.00 0.000
2     1  0.25 0.363
3     1  0.50 0.914
4     1  1.00 1.120
5     1  2.00 2.280
6     1  3.00 1.630
```

Listing 8:

```
> pk <- as.keyed(pk, key=c('SUBJ', 'HOUR'))
> head(pk)
```

```
  SUBJ HOUR    DV
1     1  0.00 0.000
2     1  0.25 0.363
3     1  0.50 0.914
4     1  1.00 1.120
5     1  2.00 2.280
6     1  3.00 1.630
```

Listing 9:

```
> summary(pk)
```

```
SUBJ~HOUR
1 NA keys
2 duplicate keys
unsorted: 2
```

Listing 10:

```
> pk[naKeys(pk),]
```

```
  SUBJ HOUR    DV
561   40    NA 100
```

Listing 11:

```
> pk[dupKeys(pk),]
```

	SUBJ	HOUR	DV
560	40	72	35.5
562	40	72	NA

Listing 12:

```
> !pk
```

	SUBJ	HOUR	DV
560	40	72	35.5
561	40	NA	100.0
562	40	72	NA

Listing 13:

```
> bad <- pk[with(pk, is.na(HOUR) | is.na(DV)),]
> bad
```

	SUBJ	HOUR	DV
561	40	NA	100
562	40	72	NA

Listing 14:

```
> pk <- pk - bad
> summary(pk)
```

```
SUBJ~HOUR
0 NA keys
0 duplicate keys
```

Looks okay.

Combine these data sources into an NMTRAN-style data set. The function ‘aug’ adds columns on-the-fly. The function ‘as.nm’ sets up a chain reaction that makes sure the final result has properties of an NMTRAN data set as described in ?nm.

Every source must specify DATETIME or HOUR. All of ours specify HOUR. If HOUR is the same for two records, we want, e.g., pk samples to sort before dose records (assumed predose). SEQ controls the sort order when times and subject identifiers match.

The plus operator means “outer join” or “full merge” when the arguments are “keyed” data.frames. The pipe operator means “left join” (merge, all.x=TRUE) when the arguments are “keyed” data.frames.

Listing 15:

```
> dat <- as.nm(
+   aug(dose, SEQ=1, EVID=1) +
+   aug(pk, SEQ=0, EVID=0) |
+   dem
+ )
> summary(dat)
```

```

      value
rows      600
records   600
comments    0
subjects   40
longestCase 72
naKeys      0
dupKeys     0
badDv       0
falseDv     0
zeroDv      25
predoseDv   40
badAmt      0
falseAmt    0
zeroAmt     0
noPk        0
badII       0

```

Note predose/zero DV. See ?zeroDv We comment-out these records.

Listing 16:

```

> dat <- hide(dat, where=predoseDv(dat), why='predose')
> summary(dat)

```

```

      value
rows      600
records   560
comments   40
subjects   40
longestCase 72
naKeys      0
dupKeys     0
badDv       0
falseDv     0
zeroDv      10
predoseDv   0
badAmt      0
falseAmt    0
zeroAmt     0
noPk        0
badII       0

```

We still have some zero DV that are not predose. We comment those as well.

Listing 17:

```

> dat <- hide(dat, where=zeroDv(dat), why='zerodv')
> summary(dat)

```

```

      value
rows      600

```

```
records      550
comments     50
subjects     40
longestCase  72
naKeys       0
dupKeys      0
badDv        0
falseDv      0
zeroDv       0
predoseDv    0
badAmt       0
falseAmt     0
zeroAmt      0
noPk         0
badII        0
```

Listing 18:

```
> head(dat)
```

	C	SUBJ	TIME	SEQ	HOUR	EVID	AMT	DV	HEIGHT	WEIGHT	SEX	AGE	DOSE	FED	SMK	DS
1	C	1	0.00	0	0.00	0	NA	0.000	174	74.2	0	29.1	1000	1	0	0
2	.	1	0.00	1	0.00	1	1000	NA	174	74.2	0	29.1	1000	1	0	0
3	.	1	0.25	0	0.25	0	NA	0.363	174	74.2	0	29.1	1000	1	0	0
4	.	1	0.50	0	0.50	0	NA	0.914	174	74.2	0	29.1	1000	1	0	0
5	.	1	1.00	0	1.00	0	NA	1.120	174	74.2	0	29.1	1000	1	0	0
6	.	1	2.00	0	2.00	0	NA	2.280	174	74.2	0	29.1	1000	1	0	0

  

	CRCN	ID	TAFD	TAD	LDOS	MDV	predose	zerodv
1	83.5	1	0.00	NA	NA	0	1	0
2	83.5	1	0.00	0.00	1000	1	0	0
3	83.5	1	0.25	0.25	1000	0	0	0
4	83.5	1	0.50	0.50	1000	0	0	0
5	83.5	1	1.00	1.00	1000	0	0	0
6	83.5	1	2.00	2.00	1000	0	0	0

We could rearrange columns for convenience and clarity.

Listing 19:

```
> dat <- shuffle(dat,c('C','ID','TIME','SEQ','EVID','AMT','DV'))
> head(dat)
```

	C	ID	TIME	SEQ	EVID	AMT	DV	SUBJ	HOUR	HEIGHT	WEIGHT	SEX	AGE	DOSE	FED	SMK
1	C	1	0.00	0	0	NA	0.000	1	0.00	174	74.2	0	29.1	1000	1	0
2	.	1	0.00	1	1	1000	NA	1	0.00	174	74.2	0	29.1	1000	1	0
3	.	1	0.25	0	0	NA	0.363	1	0.25	174	74.2	0	29.1	1000	1	0
4	.	1	0.50	0	0	NA	0.914	1	0.50	174	74.2	0	29.1	1000	1	0
5	.	1	1.00	0	0	NA	1.120	1	1.00	174	74.2	0	29.1	1000	1	0
6	.	1	2.00	0	0	NA	2.280	1	2.00	174	74.2	0	29.1	1000	1	0

  

	DS	CRCN	TAFD	TAD	LDOS	MDV	predose	zerodv
1	0	83.5	0.00	NA	NA	0	1	0

```
2  0 83.5 0.00 0.00 1000  1      0      0
3  0 83.5 0.25 0.25 1000  0      0      0
4  0 83.5 0.50 0.50 1000  0      0      0
5  0 83.5 1.00 1.00 1000  0      0      0
6  0 83.5 2.00 2.00 1000  0      0      0
```

We create a file using write.nm to format NAs specially, etc.

Listing 20:

```
> write.nm(dat, file='../data/derived/phase1.csv')
```

We create a summary of which columns were hidden for which reasons.

Listing 21:

```
> summary(hidden(dat))
```

```
      predose zerodv
total      40      10
unique      40      10
```