

Parameter Table

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1 Purpose

This script picks up after model.Rnw to process bootstrap results and make a parameter table.

1.1 Package

Listing 1:

```
> getwd()

[1] "/home/timb/metrumrg/inst/sample/script"
```

Listing 2:

```
> require(metrumrg)

metrumrg 5.0
```

2 Parameter Table

Listing 3:

```
> tab <- wikipab(1005,'../nonmem')
> tab

  parameter      description
1   THETA1      apparent oral clearance
2   THETA2      central volume of distribution
3   THETA3      absorption rate constant
4   THETA4      intercompartmental clearance
5   THETA5      peripheral volume of distribution
6   THETA6      male effect on clearance
```

```

7      THETA7              weight effect on clearance
8      OMEGA1.1            interindividual variability of clearance
9      OMEGA2.2            interindividual variability of central volume
10     OMEGA3.3            interindividual variability of Ka
11     SIGMA1.1            proportional error

                                model tool  run
1  CL/F (L/h) ~ theta_1 *  theta_6 ^MALE * (WT/70)^theta_7 * e^eta_1  nm7 1005
2                                V_c /F (L) ~ theta_2 * (WT/70)^1 * e^eta_2  nm7 1005
3                                K_a (h^-1 ) ~ theta_3 * e^eta_3  nm7 1005
4                                Q/F (L/h) ~ theta_4  nm7 1005
5                                V_p /F (L) ~ theta_5  nm7 1005
6                                MALE_CL/F ~ theta_6  nm7 1005
7                                WT_CL/F ~ theta_7  nm7 1005
8                                IIV_CL/F ~ Omega_1.1  nm7 1005
9                                IIV_V_c /F ~ Omega_2.2  nm7 1005
10                               IIV_K_a ~ Omega_3.3  nm7 1005
11                               err_prop ~ Sigma_1.1  nm7 1005

      estimate prse          se
1      8.57997 9.53      0.817948
2      21.6409 9.34      2.02094
3      0.0684281 8.04 0.00550178
4       3.78411 13.5      0.511271
5      107.376 15.7      16.8344
6       0.998986 14.8      0.148279
7       1.67117 21.7      0.363297
8       0.195776 23      0.0450967
9       0.128574 30.4      0.0391104
10      0.106527 25.3      0.0268981
11      0.067111 11.4      0.00766169

```

Listing 4:

```

> tab$estimate <- as.character(signif(as.numeric(tab$estimate),3))
> tab$estimate <- with(tab, paste(estimate,'$',justUnits(model),'$'))
> tab$name <- with(tab, wiki2label(model))

```

```
> tab$root <- signif(sqrt(exp(text2decimal(tab$estimate))-1),3)*100
> needcv <- contains('OMEGA|SIGMA',tab$parameter)
> tab <- within(tab, estimate[needcv] <- paste(estimate[needcv],parens(glue('\\%CV=',root[needcv]))))
> tab$root <- NULL
> #offdiag <- contains('2.1',tab$parameter)
> #tab$estimate[offdiag] <- text2decimal(tab$estimate[offdiag])
> #omegablock <- text2decimal(tab$estimate[contains('Omega..(1|2)',tab$parameter)])
> #cor <- signif(half(cov2cor(as.matrix(as.halfmatrix(omegablock))))[[2]],3)
> #tab$estimate[offdiag] <- paste(sep=',',tab$estimate[offdiag], ' (COR=',cor,')')
> tab$model[is.na(tab$model)] <- ''
> boot <- read.csv('../nonmem/1005.boot/log.csv',as.is=TRUE)
> boot <- boot[boot$moment=='estimate',]
> boot <- data.frame(cast(boot,... ~ moment))
> boot[] <- lapply(boot,as.character)
> boot <- boot[contains('THETA|OMEGA|SIGMA',boot$parameter),c('parameter','estimate')]
> boot$estimate <- as.numeric(boot$estimate)
> boot <-data.frame(
+   cast(
+     boot,
+     parameter ~ .,
+     value='estimate',
+     fun=function(x)list(
+       lo=as.character(
+         signif(
+           quantile(
+             x,
+             probs=0.05,
+             na.rm=TRUE
+           ),
+           3
+         )
+       ),
+       hi=as.character(
+         signif(
```

```
+      quantile(
+      x,
+      probs=0.95,
+      na.rm=TRUE
+      ),
+      3
+    )
+  )
+ )
+ )
+ )
+ )
> boot$CI <- with(boot, parens(glue(lo,',',hi)))
> tab <- stableMerge(tab,boot[,c('parameter','CI')])
> tab <- within(tab, se <- name <- run <- tool <- parameter <- NULL)
> tab$model <- wiki2latex(noUnits(tab$model))
> tab
```

	description	model
1	apparent oral clearance	$\text{CL/F} \sim \theta_1 \cdot \theta_6^{\text{MALE}} \cdot (\text{WT}/70)^{\theta_7} \cdot e^{\eta_1}$
2	central volume of distribution	$\text{V}_c/\text{F} \sim \theta_2 \cdot (\text{WT}/70)^{\theta_1} \cdot e^{\eta_2}$
3	absorption rate constant	$\text{K}_a \sim \theta_3 \cdot e^{\eta_3}$
4	intercompartmental clearance	$\text{Q/F} \sim \theta_4$
5	peripheral volume of distribution	
6	male effect on clearance	
7	weight effect on clearance	
8	interindividual variability of clearance	
9	interindividual variability of central volume	
10	interindividual variability of K_a	
11	proportional error	

5					$\mathrm{V}_{\{p\}}/F \sim \theta_{\{5\}}$
6					$\mathrm{MALE}_{\{CL/F\}} \sim \theta_{\{6\}}$
7					$\mathrm{WT}_{\{CL/F\}} \sim \theta_{\{7\}}$
8					$\mathrm{IIV}_{\{CL/F\}} \sim \Omega_{\{1.1\}}$
9					$\mathrm{IIV}_{\{V_{\{c\}}/F\}} \sim \Omega_{\{2.2\}}$
10					$\mathrm{IIV}_{\{K_{\{a\}}\}} \sim \Omega_{\{3.3\}}$
11					$\mathrm{err}_{\{prop\}} \sim \Sigma_{\{1.1\}}$

		estimate	prse		CI
1		8.58	\$ L/h \$	9.53	(7.17, 9.98)
2		21.6	\$ L \$	9.34	(18.2, 25.2)
3		0.0684	\$ h ⁻¹ \$	8.04	(0.0593, 0.078)
4		3.78	\$ L/h \$	13.5	(3.03, 4.77)
5		107	\$ L \$	15.7	(84.8, 164)
6		0.999	\$ \$	14.8	(0.773, 1.31)
7		1.67	\$ \$	21.7	(1.02, 2.3)
8	0.196	\$ \$	(\%CV=46.5)	23	(0.124, 0.266)
9	0.129	\$ \$	(\%CV=37.1)	30.4	(0.064, 0.187)
10	0.107	\$ \$	(\%CV=33.6)	25.3	(0.064, 0.152)
11	0.0671	\$ \$	(\%CV=26.3)	11.4	(0.0551, 0.08)

Table 1: Parameter Estimates from Population Pharmacokinetic Model Run 1005

description	model	estimate	prse	CI
apparent oral clearance	$CL/F \sim \theta_1 \cdot \theta_6^{MALE} \cdot (WT/70)^{\theta_7} \cdot e^{\eta_1}$	8.58 L/h	9.53	(7.17,9.98)
central volume of distribution	$V_c/F \sim \theta_2 \cdot (WT/70)^1 \cdot e^{\eta_2}$	21.6 L	9.34	(18.2,25.2)
absorption rate constant	$K_a \sim \theta_3 \cdot e^{\eta_3}$	0.0684 h ⁻¹	8.04	(0.0593,0.078)
intercompartmental clearance	$Q/F \sim \theta_4$	3.78 L/h	13.5	(3.03,4.77)
peripheral volume of distribution	$V_p/F \sim \theta_5$	107 L	15.7	(84.8,164)
male effect on clearance	$MALE_{CL/F} \sim \theta_6$	0.999	14.8	(0.773,1.31)
weight effect on clearance	$WT_{CL/F} \sim \theta_7$	1.67	21.7	(1.02,2.3)
interindividual variability of clearance	$IIV_{CL/F} \sim \Omega_{1.1}$	0.196 (%CV=46.5)	23	(0.124,0.266)
interindividual variability of central volume	$IIV_{V_c/F} \sim \Omega_{2.2}$	0.129 (%CV=37.1)	30.4	(0.064,0.187)
interindividual variability of Ka	$IIV_{K_a} \sim \Omega_{3.3}$	0.107 (%CV=33.6)	25.3	(0.064,0.152)
proportional error	$err_{prop} \sim \Sigma_{1.1}$	0.0671 (%CV=26.3)	11.4	(0.0551,0.08)