MS 2007-0162-RRR
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Supplemental Materials
(to be posted on the Web)

Table 5: When both SEM_BK and PS_AIR assumptions hold.

5.a. Mplus input for data generation

```
title: Data generation (true) model for Table 4
       All the assumptions of the SEM_BK and PS_AIR models hold. That is,
       exclusion restriction, monotonicity, ignorability, constant effect hold.
       See Table 2 for PS parameters considered in data generation.

montecarlo:
      names = y z; ! y is a continuous outcome.
      nobservations = 500; ! N=500 in each data set.
      nreps = 500; !500 data sets generated.
      cutpoints = z(0); ! z is the intervention assignment.
                        ! split at zero in the normal distribution.
                        ! 50% control, 50% intervention.
      genclasses = c(3); ! Under monotonicity, 3 principal strata are generated.
      classes = c(1); ! analysis is done assuming one class.
      repsave = all; ! all 500 data sets will be saved.
      save = all*.dat; ! each data set has a name starting with all.

model population: ! data generation model.
      %overall%
       [y*1];  ! generate the outcome.
        y*1;   ! normally distributed with mean=1 and variance=1.
       [z*1];  ! generate an intervention assignment variable.
        z*0;   ! normally distributed with mean=0 and variance=1.
               ! this variable is dichotomized (see cutpoints command).
      y on z*0.2; ! the overall treatment assignment effect = 0.2.

     [c#1*0.693147]; ! multinomial logit intercepts
     [c#2*0.693147]; ! to match true principal stratum proportions (0.4,0.4,0.2).

      %c#1% ! never-improver
          [y*1] ; ! mean outcome for never-improvers under the control condition.
           y on z*.0; ! treatment assignment effect for never-improvers = 0.
      %c#2% ! forward-improver
          [y*1] ; ! mean outcome for forward-improvers under the control condition.
           y on z*.5; ! treatment assignment effect for forward-improvers = 0.5.
      %c#3% ! always-improver
          [y*1.5] ; ! mean outcome for always-improvers under the control condition.
           y on z*.0; ! treatment assignment effect for always-improvers = 0.

 Analysis: ! data generation model.
      type = mixture ; ! data are analyzed assuming a mixture distribution.
                       ! for Table 4, analyses done here are not necessary.
                       ! necessary only to complete data generation in Mplus.
 model:
        %overall%
       y on z*0.2; ! total effect of treatment assignment estimated.
                  ! existence of 3 principal strata is ignored (see classes=1 command).
```

Table 5

5.b. **Mplus input for SEM_BK model**

```
title: Monte Carlo simulation using externally generated data.
data:   file is alllist.dat; type=montecarlo; ! read in 500 data sets from 4.a
variable: names are y z c3; ! c3 is principal stratum class, z is treatment assignment.
          usev  are y z m;  ! observed mediator created based on c3 and z (see below).
define: if (c3==1 and z==1)  then m=0;
        if (c3==1 and z==0)  then m=0;
        if (c3==2 and z==1)  then m=1;
        if (c3==2 and z==0)  then m=0;
        if (c3==3 and z==1)  then m=1;
        if (c3==3 and z==0)  then m=1;

model: ! SEM_BK analysis model
      y on z*0 (c); ! SEM parameter c. true values specified on the right side of *
                    ! so that coverage rates can be calculated.
      y on m*.5 (b); ! SEM parameter b.
      m on z*.4 (a); ! SEM parameter a.
     [m*0.2] (alpha_m); ! SEM parameter alpha_m.

model constraint: ! this command lets us create new parameters using the parameters
                  ! specified in model command above.
            new(ab*.2 ga_n*.0 ga_f*.5 ga_b ga_a*.0
                pi_n*.4 pi_f*.4 pi_a*.2); ! true values assigned to the new parameters.
            ab= a*b; ! SEM parameter ab.

           ! from here, SEM parameters are translated into PS parameters.
            ga_n = c; ! Eq. (25).
            ga_f = b + c; ! Eq. (27) and constant effect.
            ga_b =-b + c; ! Eq. (31).
            ga_a = c; ! Eq. (26) and constant effect.
            pi_f = a; ! Eq. (28) and monotonicity.
            pi_a = alpha_m; ! Eq. (29) and monotonicity.
            pi_n=1-pi_f-pi_a; ! Eq. (30) and monotonicity.
```

Table 5
5.c. **Mplus input for PS_AIR model**

```
title:  Monte Carlo simulation using externally generated data.
data:   file is alllist.dat;  type=montecarlo;
variable:   names are  y z c3;
              usev are y z m;
define: if (c3==1 and z==1)  then m=0;
        if (c3==1 and z==0)  then m=0;
        if (c3==2 and z==1)  then m=1;
        if (c3==2 and z==0)  then m=0;
        if (c3==3 and z==1)  then m=1;
        if (c3==3 and z==0)  then m=1;

model: ! PS_AIR analysis model
      y on z*0.2 (gamma_t); ! the overall (total) treatment assignment effect.
      m on z*0.4 (pi_f); ! PS parameter pi_f.
     [m*0.2] (pi_a); ! PS parameter pi_a.

     model constraint:
            new(gamma_f*0.5 pi_n*0.4 a*0.4 b*0.5 ab*0.2);
            pi_n=1-pi_f-pi_a; ! Eq. (8).
            gamma_f=gamma_t/pi_f; ! Eq. (10).

          ! from here, PS parameters are translated into SEM parameters.
            a=pi_f; ! Eq. (23) and monotonicity.
            b=gamma_f; ! Eq. (22) and exclusion restriction.
            ab=a*b;
```

Table 9: When none of the SEM_BK and PS_AIR assumptions hold.

9.a. Mplus input for data generation

```
title: Data generation (true) model for Table 8
       None of the assumptions of the SEM_BK and PS_AIR models hold.
       See Table 2 for PS parameters considered in data generation.

montecarlo:
      names = y z; ! y is a continuous outcome.
      nobservations = 500; ! N=500 in each data set.
      nreps = 500; !500 data sets generated.
      cutpoints = z(0); ! z is the intervention assignment.
                        ! split at zero in the normal distribution.
                        ! 50% control, 50% intervention.
      genclasses = c(4); ! 4 principal strata are generated.
      classes = c(1); ! analysis is done assuming one class.
      repsave = all; ! all 500 data sets will be saved.
      save = none*.dat; ! each data set has a name starting with none.

model population: ! data generation model.
      %overall%
       [y*1];  ! generate the outcome.
        y*1;   ! normally distributed with mean=1 and variance=1.
       [z*1];  ! generate an intervention assignment variable.
        z*0;   ! normally distributed with mean=0 and variance=1.
               ! this variable is dichotomized (see cutpoints command).
      y on z*0.15; ! the overall treatment assignment effect = 0.15.

     [c#1*0.405465]; ! multinomial logit intercepts
     [c#2*-0.69315]; ! to match true principal stratum proportions (0.3,0.4,0.1,0.2).
     [c#3*0.693150];

      %c#1% ! never-improver
          [y*1] ; ! mean outcome for never-improvers under the control condition.
           y on z*-.1; ! treatment assignment effect for never-improvers = -0.1.
      %c#2% ! backward-improver
          [y*1] ; ! mean outcome for backward-improvers under the control condition.
           y on z*-.4; ! treatment assignment effect for never-improvers = -0.4.
      %c#3% ! forward-improver
          [y*1.2] ; ! mean outcome for forward-improvers under the control condition.
           y on z*.5; ! treatment assignment effect for forward-improvers = 0.5.
      %c#4% ! always-improver
          [y*1.6] ; ! mean outcome for always-improvers under the control condition.
           y on z*.2; ! treatment assignment effect for always-improvers = 0.2.

 Analysis: ! data generation model.
      type = mixture ; ! data are analyzed assuming a mixture distribution.
                       ! for Table 8, analyses done here are not necessary.
                       ! necessary only to complete data generation in Mplus.
 model:
        %overall%
       y on z*0.15 ; ! total effect of treatment assignment estimated.
                   ! existence of 4 principal strata is ignored (see classes=1 command).
```

Table 9

9.b. **Mplus input for SEM_BK model**

```
title: Monte Carlo simulation using externally generated data.
data:   file is nonelist.dat; type=montecarlo; ! read in 500 data sets from 4.a
variable: names are y z c4; ! c4 is principal stratum class, z is treatment assignment.
          usev  are y z m;  ! observed mediator created based on c4 and z (see below).
  define: if (c4==1 and z==1)  then m=0;
          if (c4==1 and z==0)  then m=0;
          if (c4==2 and z==1)  then m=0;
          if (c4==2 and z==0)  then m=1;
          if (c4==3 and z==1)  then m=1;
          if (c4==3 and z==0)  then m=0;
          if (c4==4 and z==1)  then m=1;
          if (c4==4 and z==0)  then m=1;

model: ! SEM_BK analysis model
      y on z*-.1 (c); ! SEM parameter c. true values specified on the right side of *
                      ! so that coverage rates can be calculated.
      y on m*.3 (b); ! SEM parameter b.
      m on z*.3 (a); ! SEM parameter a.
     [m*0.2] (alpha_m); ! SEM parameter alpha_m.

model constraint: ! this command lets us create new parameters using the parameters
                  ! specified in model command above.
            new(ab*.09 ga_n*-.1 ga_f*.5 ga_b*-.4 ga_a*.2
                pi_n*.3 pi_f*.4 pi_a*.2); ! true values assigned to the new parameters.
            ab= a*b; ! SEM parameter ab.

            ! from here, SEM parameters are translated into PS parameters.
            ga_n = c; ! Eq. (25).
            ga_f = b + c; ! Eq. (27) and constant effect.
            ga_b =-b + c; ! Eq. (31).
            ga_a = c; ! Eq. (26) and constant effect.
            pi_f = a; ! Eq. (28) and monotonicity.
            pi_a = alpha_m; ! Eq. (29) and monotonicity.
            pi_n=1-pi_f-pi_a; ! Eq. (30) and monotonicity.
```

Table 9
9.c. **Mplus input for PS_AIR model**

```
title:  Monte Carlo simulation using externally generated data.
data:   file is nonelist.dat;  type=montecarlo;
variable:   names are  y z c4;
            usev are y z m;
define: if (c4==1 and z==1)  then m=0;
          if (c4==1 and z==0)  then m=0;
          if (c4==2 and z==1)  then m=0;
          if (c4==2 and z==0)  then m=1;
          if (c4==3 and z==1)  then m=1;
          if (c4==3 and z==0)  then m=0;
          if (c4==4 and z==1)  then m=1;
          if (c4==4 and z==0)  then m=1;

model: ! PS_AIR analysis model
      y on z*0.15 (gamma_t); ! the overall (total) treatment assignment effect.
      m on z*0.4 (pi_f); ! PS parameter pi_f.
     [m*0.2] (pi_a); ! PS parameter pi_a.

     model constraint:
            new(gamma_f*0.5 pi_n*0.3 a*0.3 b*0.3 ab*0.09);
            pi_n=1-pi_f-pi_a; ! Eq. (8).
            gamma_f=gamma_t/pi_f; ! Eq. (10).

          ! from here, PS parameters are translated into SEM parameters.
            a=pi_f; ! Eq. (23) and monotonicity.
            b=gamma_f; ! Eq. (22) and exclusion restriction.
            ab=a*b;
```

Table 9

9.d. **Mplus input for SEM_Mac (PS_Ig) model**

```
title:  Monte Carlo simulation using externally generated data.
data:   file is nonelist.dat;  type=montecarlo;
variable:   names are  y z c4;
            usev are y z m mz; ! interaction parameter is included in the analyses.
define: if (c4==1 and z==1)  then m=0;
          if (c4==1 and z==0)  then m=0;
          if (c4==2 and z==1)  then m=0;
          if (c4==2 and z==0)  then m=1;
          if (c4==3 and z==1)  then m=1;
          if (c4==3 and z==0)  then m=0;
          if (c4==4 and z==1)  then m=1;
          if (c4==4 and z==0)  then m=1;
          mz = m*z; ! interaction parameter is created based on m and z

model: ! SEM_Mac analysis model
      y on z*-.1 (c); ! SEM parameter c. true values specified on the right side of *
                    ! so that coverage rates can be calculated.
      y on m*.3 (b); ! SEM parameter b.
      y on mz*.09 (d); ! SEM parameter d.
      m on z*.3 (a); ! SEM parameter a.
     [m*0.2] (alpha_m); ! SEM parameter alpha_m.

model constraint:
            new(ga_n*-.1 ga_f*.5 ga_b*-.4 ga_a*.2
                pi_n*.3 pi_f*.4 pi_a*.2); ! true values assigned to the new parameters.
            ab= a*b; ! SEM parameter ab.

            ! from here, SEM parameters are translated into PS parameters.
            ga_n = c; ! Eq. (25).
            ga_f = b + c + d; ! Eq. (27).
            ga_b =-b + c; ! Eq. (31).
            ga_a = c + d; ! Eq. (26).
            pi_f = a; ! Eq. (28) and monotonicity.
            pi_a = alpha_m; ! Eq. (29) and monotonicity.
            pi_n=1-pi_f-pi_a; ! Eq. (30) and monotonicity.
```