

Computations on case 3. Three-period design using non-concurrent controls

We first define the treatment effect for arm 2 following the expressions presented in the supplementary material (see Section A.2). To do so, we define the matrices A, B, and C, and use equation (1.b) to obtain point estimates

```
In[*]:= nd1 = n01 + n11
nd2 = n02 + n12 + n22
nd3 = n03 + n23
A = {{nd1, 0, 0}, {0, nd2, 0}, {0, 0, nd3}}
B = {{n11, 0}, {n12, n22}, {0, n23}}
Cm = {{n11 + n12, 0}, {0, n22 + n23}}

Out[*]:= n01 + n11

Out[*]:= n02 + n12 + n22

Out[*]:= n03 + n23

Out[*]:= {{n01 + n11, 0, 0}, {0, n02 + n12 + n22, 0}, {0, 0, n03 + n23}}

Out[*]:= {{n11, 0}, {n12, n22}, {0, n23}}

Out[*]:= {{n11 + n12, 0}, {0, n22 + n23}}

In[*]:= M = FullSimplify[Inverse[Cm - Transpose[B].Inverse[A].B]]
Nm = {{n11 * theta11 + n12 * theta12}, {n22 * theta22 + n23 * theta23}}
Collect[FullSimplify[M.Nm][[2]], {theta11, theta12, theta22, theta23}]
w11 = (n11 (n01 + n11) n12 n22 (n03 + n23) ) /
      (n11 n12 (n02 n03 n22 + n03 n22 n23 + n02 (n03 + n22) n23) +
       n01 (n03 n11 n12 n22 + (n03 n11 n12 + n11 n12 n22 + n03 (n11 + n12) n22) n23 +
        n02 (n11 + n12) (n22 n23 + n03 (n22 + n23) )))
w12 = ((n01 + n11) n12^2 n22 (n03 + n23) ) /
      (n11 n12 (n02 n03 n22 + n03 n22 n23 + n02 (n03 + n22) n23) +
       n01 (n03 n11 n12 n22 + (n03 n11 n12 + n11 n12 n22 + n03 (n11 + n12) n22) n23 +
        n02 (n11 + n12) (n22 n23 + n03 (n22 + n23) )))
w22 =
      (n22 (n11 n12 (n02 + n22) + n01 (n11 n12 + n02 (n11 + n12) + (n11 + n12) n22) ) (n03 + n23) ) /
      (n11 n12 (n02 n03 n22 + n03 n22 n23 + n02 (n03 + n22) n23) +
       n01 (n03 n11 n12 n22 + (n03 n11 n12 + n11 n12 n22 + n03 (n11 + n12) n22) n23 +
        n02 (n11 + n12) (n22 n23 + n03 (n22 + n23) )))
w23 =
      ((n11 n12 (n02 + n22) + n01 (n11 n12 + n02 (n11 + n12) + (n11 + n12) n22) ) n23 (n03 + n23) ) /
      (n11 n12 (n02 n03 n22 + n03 n22 n23 + n02 (n03 + n22) n23) +
       n01 (n03 n11 n12 n22 + (n03 n11 n12 + n11 n12 n22 + n03 (n11 + n12) n22) n23 +
        n02 (n11 + n12) (n22 n23 + n03 (n22 + n23) )))
sol = M.Nm
True ==
FullSimplify[sol[[2]][[1]] == w11 * theta11 + w12 * theta12 + w22 * theta22 + w23 * theta23]
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$$\begin{aligned}
Out[*]= & \{ \{ ((n01 + n11) (n03 (n02 + n12) n22 + n03 (n02 + n12) n23 + (n02 + n03 + n12) n22 n23)) / \\
& (n01 n03 (n11 n12 + n02 (n11 + n12)) n22 + \\
& n01 (n03 n11 n12 + n11 n12 n22 + n03 (n11 + n12) n22 + n02 (n11 + n12) (n03 + n22)) n23 + \\
& n11 n12 (n02 n03 n22 + n03 n22 n23 + n02 (n03 + n22) n23)) , \\
& ((n01 + n11) n12 n22 (n03 + n23)) / (n11 n12 (n02 n03 n22 + n03 n22 n23 + n02 (n03 + n22) n23) + \\
& n01 (n03 n11 n12 n22 + (n03 n11 n12 + n11 n12 n22 + n03 (n11 + n12) n22) n23 + \\
& n02 (n11 + n12) (n22 n23 + n03 (n22 + n23)))) \} , \\
& \{ ((n01 + n11) n12 n22 (n03 + n23)) / (n11 n12 (n02 n03 n22 + n03 n22 n23 + n02 (n03 + n22) n23) + \\
& n01 (n03 n11 n12 n22 + (n03 n11 n12 + n11 n12 n22 + n03 (n11 + n12) n22) n23 + \\
& n02 (n11 + n12) (n22 n23 + n03 (n22 + n23)))) , \\
& ((n11 n12 (n02 + n22) + n01 (n11 n12 + n02 (n11 + n12) + (n11 + n12) n22)) (n03 + n23)) / \\
& (n11 n12 (n02 n03 n22 + n03 n22 n23 + n02 (n03 + n22) n23) + \\
& n01 (n03 n11 n12 n22 + (n03 n11 n12 + n11 n12 n22 + n03 (n11 + n12) n22) n23 + \\
& n02 (n11 + n12) (n22 n23 + n03 (n22 + n23)))) \} \}
\end{aligned}$$

$$Out[*]= \{ \{ n11 \theta_{11} + n12 \theta_{12} \}, \{ n22 \theta_{22} + n23 \theta_{23} \} \}$$

$$\begin{aligned}
Out[*]= & \{ (n11 (n01 + n11) n12 n22 (n03 + n23) \theta_{11}) / \\
& (n11 n12 (n02 n03 n22 + n03 n22 n23 + n02 (n03 + n22) n23) + \\
& n01 (n03 n11 n12 n22 + (n03 n11 n12 + n11 n12 n22 + n03 (n11 + n12) n22) n23 + \\
& n02 (n11 + n12) (n22 n23 + n03 (n22 + n23)))) + \\
& ((n01 + n11) n12^2 n22 (n03 + n23) \theta_{12}) / \\
& (n11 n12 (n02 n03 n22 + n03 n22 n23 + n02 (n03 + n22) n23) + \\
& n01 (n03 n11 n12 n22 + (n03 n11 n12 + n11 n12 n22 + n03 (n11 + n12) n22) n23 + \\
& n02 (n11 + n12) (n22 n23 + n03 (n22 + n23)))) + \\
& (n22 (n11 n12 (n02 + n22) + n01 (n11 n12 + n02 (n11 + n12) + (n11 + n12) n22)) \\
& (n03 + n23) \theta_{22}) / (n11 n12 (n02 n03 n22 + n03 n22 n23 + n02 (n03 + n22) n23) + \\
& n01 (n03 n11 n12 n22 + (n03 n11 n12 + n11 n12 n22 + n03 (n11 + n12) n22) n23 + \\
& n02 (n11 + n12) (n22 n23 + n03 (n22 + n23)))) + \\
& ((n11 n12 (n02 + n22) + n01 (n11 n12 + n02 (n11 + n12) + (n11 + n12) n22)) \\
& n23 (n03 + n23) \theta_{23}) / \\
& (n11 n12 (n02 n03 n22 + n03 n22 n23 + n02 (n03 + n22) n23) + \\
& n01 (n03 n11 n12 n22 + (n03 n11 n12 + n11 n12 n22 + n03 (n11 + n12) n22) n23 + \\
& n02 (n11 + n12) (n22 n23 + n03 (n22 + n23)))) \}
\end{aligned}$$

$$\begin{aligned}
Out[*]= & (n11 (n01 + n11) n12 n22 (n03 + n23)) / \\
& (n11 n12 (n02 n03 n22 + n03 n22 n23 + n02 (n03 + n22) n23) + \\
& n01 (n03 n11 n12 n22 + (n03 n11 n12 + n11 n12 n22 + n03 (n11 + n12) n22) n23 + \\
& n02 (n11 + n12) (n22 n23 + n03 (n22 + n23))))
\end{aligned}$$

$$\begin{aligned}
Out[*]= & ((n01 + n11) n12^2 n22 (n03 + n23)) / (n11 n12 (n02 n03 n22 + n03 n22 n23 + n02 (n03 + n22) n23) + \\
& n01 (n03 n11 n12 n22 + (n03 n11 n12 + n11 n12 n22 + n03 (n11 + n12) n22) n23 + \\
& n02 (n11 + n12) (n22 n23 + n03 (n22 + n23))))
\end{aligned}$$

$$\begin{aligned}
Out[*]= & (n22 (n11 n12 (n02 + n22) + n01 (n11 n12 + n02 (n11 + n12) + (n11 + n12) n22)) (n03 + n23)) / \\
& (n11 n12 (n02 n03 n22 + n03 n22 n23 + n02 (n03 + n22) n23) + \\
& n01 (n03 n11 n12 n22 + (n03 n11 n12 + n11 n12 n22 + n03 (n11 + n12) n22) n23 + \\
& n02 (n11 + n12) (n22 n23 + n03 (n22 + n23))))
\end{aligned}$$

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Out[ ]= ( (n11 n12 (n02 + n22) + n01 (n11 n12 + n02 (n11 + n12) + (n11 + n12) n22) ) n23 (n03 + n23) ) /
(n11 n12 (n02 n03 n22 + n03 n22 n23 + n02 (n03 + n22) n23) +
n01 (n03 n11 n12 n22 + (n03 n11 n12 + n11 n12 n22 + n03 (n11 + n12) n22) n23 +
n02 (n11 + n12) (n22 n23 + n03 (n22 + n23) ) ) )

Out[ ]= { { ( (n01 + n11) (n03 (n02 + n12) n22 + n03 (n02 + n12) n23 + (n02 + n03 + n12) n22 n23)
(n11 theta11 + n12 theta12) ) / (n01 n03 (n11 n12 + n02 (n11 + n12) ) n22 +
n01 (n03 n11 n12 + n11 n12 n22 + n03 (n11 + n12) n22 + n02 (n11 + n12) (n03 + n22) ) n23 +
n11 n12 (n02 n03 n22 + n03 n22 n23 + n02 (n03 + n22) n23) ) +
( (n01 + n11) n12 n22 (n03 + n23) (n22 theta22 + n23 theta23) ) /
(n11 n12 (n02 n03 n22 + n03 n22 n23 + n02 (n03 + n22) n23) +
n01 (n03 n11 n12 n22 + (n03 n11 n12 + n11 n12 n22 + n03 (n11 + n12) n22) n23 +
n02 (n11 + n12) (n22 n23 + n03 (n22 + n23) ) ) ) },
{ ( (n01 + n11) n12 n22 (n03 + n23) (n11 theta11 + n12 theta12) ) /
(n11 n12 (n02 n03 n22 + n03 n22 n23 + n02 (n03 + n22) n23) +
n01 (n03 n11 n12 n22 + (n03 n11 n12 + n11 n12 n22 + n03 (n11 + n12) n22) n23 +
n02 (n11 + n12) (n22 n23 + n03 (n22 + n23) ) ) ) +
( (n11 n12 (n02 + n22) + n01 (n11 n12 + n02 (n11 + n12) + (n11 + n12) n22) )
(n03 + n23) (n22 theta22 + n23 theta23) ) /
(n11 n12 (n02 n03 n22 + n03 n22 n23 + n02 (n03 + n22) n23) +
n01 (n03 n11 n12 n22 + (n03 n11 n12 + n11 n12 n22 + n03 (n11 + n12) n22) n23 +
n02 (n11 + n12) (n22 n23 + n03 (n22 + n23) ) ) ) } }

Out[ ]= True

```

Variance computation

To compute the variance of treatment effect 2, first note

$$\text{Var}(\text{theta2}) = \text{Var}(w11 \cdot \text{theta11} + w12 \cdot \text{theta12} + w22 \cdot \text{theta22} + w23 \cdot \text{theta23})$$

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In[ ]:= theta11 = n01 / (n01 + n11) * (y11 - y01);
theta12 = (n02 + n22) / (n02 + n12 + n22) * y12 -
  ((n02 / (n02 + n12 + n22)) * y02 + (n22 / (n02 + n12 + n22)) * y22);
theta22 = (n02 + n12) / (n02 + n12 + n22) * y22 -
  ((n02 / (n02 + n12 + n22)) * y02 + (n12 / (n02 + n12 + n22)) * y12);
theta23 = n03 / (n03 + n23) * (y23 - y03);
expr = w11 * theta11 + w12 * theta12 + w22 * theta22 + w23 * theta23;
Collect[FullSimplify[expr], {y01, y11, y02, y12, y22, y03, y23}];
expr01 = FullSimplify[
  (-n01 n03 n11 n12 n22 - n01 n11 n12 n22 n23) / (n01 n03 (n11 n12 + n02 (n11 + n12)) n22 +
    n01 (n03 n11 n12 + n11 n12 n22 + n03 (n11 + n12) n22 + n02 (n11 + n12) (n03 + n22)) n23 +
    n11 n12 (n02 n03 n22 + n03 n22 n23 + n02 (n03 + n22) n23))];
expr02 = FullSimplify[
  (-n01 n02 n03 n11 n22 - n01 n02 n03 n12 n22 - n02 n03 n11 n12 n22 - n01 n02 n11 n22 n23 -
    n01 n02 n12 n22 n23 - n02 n11 n12 n22 n23) / (n01 n03 (n11 n12 + n02 (n11 + n12)) n22 +
    n01 (n03 n11 n12 + n11 n12 n22 + n03 (n11 + n12) n22 + n02 (n11 + n12) (n03 + n22)) n23 +
    n11 n12 (n02 n03 n22 + n03 n22 n23 + n02 (n03 + n22) n23))];
expr03 = FullSimplify[
  (-n01 n03 n11 n12 n23 - n02 n03 n11 n12 n23 - n03 n11 n12 n22 n23 - n01 n03 n11 (n02 + n22)
    n23 - n01 n03 n12 (n02 + n22) n23) / (n01 n03 (n11 n12 + n02 (n11 + n12)) n22 +
    n01 (n03 n11 n12 + n11 n12 n22 + n03 (n11 + n12) n22 + n02 (n11 + n12) (n03 + n22)) n23 +
    n11 n12 (n02 n03 n22 + n03 n22 n23 + n02 (n03 + n22) n23))];
expr11 = FullSimplify[
  (n01 n03 n11 n12 n22 + n01 n11 n12 n22 n23) / (n01 n03 (n11 n12 + n02 (n11 + n12)) n22 +
    n01 (n03 n11 n12 + n11 n12 n22 + n03 (n11 + n12) n22 + n02 (n11 + n12) (n03 + n22)) n23 +
    n11 n12 (n02 n03 n22 + n03 n22 n23 + n02 (n03 + n22) n23))];
expr12 = FullSimplify[
  (-n01 n03 n11 n12 n22 - n01 n11 n12 n22 n23) / (n01 n03 (n11 n12 + n02 (n11 + n12)) n22 +
    n01 (n03 n11 n12 + n11 n12 n22 + n03 (n11 + n12) n22 + n02 (n11 + n12) (n03 + n22)) n23 +
    n11 n12 (n02 n03 n22 + n03 n22 n23 + n02 (n03 + n22) n23))];
expr22 = FullSimplify[
  (n02 n03 n11 n12 n22 + n01 n03 (n11 n12 + n02 (n11 + n12)) n22 + n01 n02 n12 n22 n23 + n02 n11
    n12 n22 n23 + n01 n11 (n02 + n12) n22 n23) / (n01 n03 (n11 n12 + n02 (n11 + n12)) n22 +
    n01 (n03 n11 n12 + n11 n12 n22 + n03 (n11 + n12) n22 + n02 (n11 + n12) (n03 + n22)) n23 +
    n11 n12 (n02 n03 n22 + n03 n22 n23 + n02 (n03 + n22) n23))];
expr23 = FullSimplify[ (n02 n03 n11 n12 n23 + n03 n11 n12 n22 n23 +
  n01 n03 (n11 n12 + n02 (n11 + n12)) + (n11 + n12) n22) n23) /
  (n01 n03 (n11 n12 + n02 (n11 + n12)) n22 +
  n01 (n03 n11 n12 + n11 n12 n22 + n03 (n11 + n12) n22 + n02 (n11 + n12) (n03 + n22)) n23 +
  n11 n12 (n02 n03 n22 + n03 n22 n23 + n02 (n03 + n22) n23))];
FullSimplify[
  Collect[FullSimplify[expr], {y01, y11, y02, y12, y22, y03, y23}] == expr01 * y01 +
    expr02 * y02 + expr03 * y03 + expr11 * y11 + expr12 * y12 + expr22 * y22 + expr23 * y23];

```

Variance expression is then $\text{term2s} \cdot \sigma^2 / N$, where

```

In[ ]:= term2f = FullSimplify[expr01^2 * y01 + expr02^2 * y02 + expr03^2 * y03 + expr11^2 * y11 +
  expr12^2 * y12 + expr22^2 * y22 + expr23^2 * y23 /. {y01 → 1 / n01, y02 → 1 / n02,
  y03 → 1 / n03, y11 → 1 / n11, y12 → 1 / n12, y22 → 1 / n22, y23 → 1 / n23}];
term2s =
  FullSimplify[term2f /. {n01 → r01 * Nt, n02 → r02 * Nt, n03 → r03 * Nt, n11 → r11 * Nt,
  n12 → r12 * Nt, n22 → r22 * Nt, n23 → r23 * Nt}] * Nt;

```

Define terms to optimise

```

In[ ]:= subst = {r11 → r1 / 2, r01 → r1 / 2, r23 → r3 / 2, r03 → r3 / 2, r02 → r2 - r12 - r22};
term1 = FullSimplify[(r11 * r01 / (r11 + r01)) + (r12 * r02 / (r12 + r02)) /. subst];
term2 = FullSimplify[(1 / term2s) /. subst];

In[ ]:= substg = {r01 → r1 - r11, r03 → r3 - r23, r02 → r2 - r12 - r22};
termg1 = FullSimplify[(r11 * r01 / (r11 + r01)) + (r12 * r02 / (r12 + r02)) /. substg];
termg2 = FullSimplify[(1 / term2s) /. substg];

```

Numerical example: optimisation assuming balanced design in periods 1 and 3

```

In[ ]:= ex = {r1 → 0.1, r2 → 0.8, r3 → 0.1};
FindMinimum[{-term1 /. ex, term1 == term2 /. ex, r12 + r22 < 0.8, r12 > 0, r22 > 0},
  {{r12, r2 / 3 /. ex}, {r22, r2 / 3 /. ex}}]

Out[ ]:= {-0.164091, {r12 → 0.24303, r22 → 0.231746}}

```

Optimisation (approach 1) - here we do not assume balanced design in periods 1 and 3 and thus also allocation rates in periods 1 and 3 are optimized

```

In[ ]:= ex = {r1 → 0.4, r2 → 0.4, r3 → 0.2};
FindMinimum[{-termg1 /. ex, termg1 == termg2 /. ex,
  r12 + r22 < 0.8, r12 > 0, r22 > 0, r11 > 0, r23 > 0, r11 < 1, r23 < 1},
  {{r11, r1 / 2 /. ex}, {r12, r2 / 3 /. ex}, {r22, r2 / 3 /. ex}, {r23, r3 / 2 /. ex}}]

Out[ ]:= {-0.144071, {r11 → 0.2, r12 → 0.0615317, r22 → 0.183165, r23 → 0.1}}

```

```

In[ ]:= FindMinimum[{-termg1 /. ex, termg1 == termg2 /. ex,
  r12 + r22 < 0.8, r12 > 0, r22 > 0, r11 > 0, r23 > 0, r11 < 1, r23 < 1},
  {{r11,  $\frac{r1}{2}$  /. ex}, {r12,  $\frac{r2}{3}$  /. ex}, { $\frac{r22}{3}$  /. ex}, {r23,  $\frac{r3}{2}$  /. ex}}]

```

FindMinimum: The variable $\frac{r22}{3}$ /. ex cannot be localized so that it can be assigned to numerical values.

```

Out[ ]:= FindMinimum[{-termg1 /. ex, termg1 == termg2 /. ex,
  r12 + r22 < 0.8, r12 > 0, r22 > 0, r11 > 0, r23 > 0, r11 < 1, r23 < 1},
  {{r11,  $\frac{r1}{2}$  /. ex}, {r12,  $\frac{r2}{3}$  /. ex}, { $\frac{r22}{3}$  /. ex}, {r23,  $\frac{r3}{2}$  /. ex}}]

```

```

In[ ]:= termg2

```

```

Out[ ]:= (r1 (-r12^2 + (r11 + r12) r2) r23^2 +
  r1 (r11 r22 (-r2 + r22) + r12 r22 (r12 - r2 + r22) + r12^2 r23 - (r11 + r12) r2 r23) r3 +
  r11^2 (-r2 r23^2 - r22^2 r3 + r2 (r22 + r23) r3)) / ((r11^2 r2 + r1 (r12^2 - (r11 + r12) r2)) r3)

```

$$\text{In}[*]:= \left\{ \left\{ r_{11}, \frac{r_1}{2} /. \text{ex} \right\}, \left\{ r_{12}, \frac{r_2}{3} /. \text{ex} \right\}, \left\{ \frac{r_{22}}{3} /. \text{ex} \right\}, \left\{ r_{23}, \frac{r_3}{2} /. \text{ex} \right\} \right\}$$

$$\text{Out}[*]:= \left\{ \{r_{11}, 0.2\}, \{r_{12}, 0.133333\}, \left\{ \frac{r_{22}}{3} \right\}, \{r_{23}, 0.1\} \right\}$$

Note that we cannot find analytical solutions, but the numerical solutions satisfy that the optimal design follows a balanced design in periods 1 and 3.

Optimisation (approach 2) - assume balanced designs in periods 1 and 3

In[*]:= constr = term1 - term2;

In[*]:= e1 = FullSimplify[Solve[D[term1, r12] == 1 D[constr, r12], 1]]

e2 = FullSimplify[Solve[D[term1, r22] == 1 D[constr, r22], 1]]

e3 = e1[[1]][[1]][[2]] == e2[[1]][[1]][[2]]

$$\text{Out}[*]:= \left\{ \left\{ 1 \rightarrow \frac{-1 + \frac{2 r_{12}}{r_2 - r_{22}}}{-1 + \frac{2 r_{12}}{r_2 - r_{22}} - \frac{8 r_{12} (r_1 + 2 r_{12}) r_{22}^2}{(r_1 r_2 + 4 r_{12} (-r_{12} + r_2))^2}} \right\} \right\}$$

$$\text{Out}[*]:= \left\{ \left\{ 1 \rightarrow \frac{r_{12}^2}{(r_2 - r_{22})^2 \left(1 + \frac{r_{12}^2}{(r_2 - r_{22})^2} - \frac{2 (r_1 + 4 r_{12}) r_{22}}{r_1 r_2 + 4 r_{12} (-r_{12} + r_2)} \right)} \right\} \right\}$$

$$\text{Out}[*]:= \frac{-1 + \frac{2 r_{12}}{r_2 - r_{22}}}{-1 + \frac{2 r_{12}}{r_2 - r_{22}} - \frac{8 r_{12} (r_1 + 2 r_{12}) r_{22}^2}{(r_1 r_2 + 4 r_{12} (-r_{12} + r_2))^2}} == \frac{r_{12}^2}{(r_2 - r_{22})^2 \left(1 + \frac{r_{12}^2}{(r_2 - r_{22})^2} - \frac{2 (r_1 + 4 r_{12}) r_{22}}{r_1 r_2 + 4 r_{12} (-r_{12} + r_2)} \right)}$$

In[*]:= sol2 = Solve[e3, {r12}];

In[*]:= solsim = Simplify[sol2[[7]]]

$$\text{Out}[*]:= \left\{ r_{12} \rightarrow \frac{1}{192 (r_2 - r_{22})} \left(32 (3 r_2^2 - 6 r_2 r_{22} + 2 r_{22}^2) + (16 i^{2^{1/3}} (i + \sqrt{3}) (3 r_2^4 - 12 r_2^3 r_{22} + 18 r_2^2 r_{22}^2 - 12 r_2 r_{22}^3 + 4 r_{22}^4 + 3 r_1 r_2 (r_2^2 - 3 r_2 r_{22} + 2 r_{22}^2))) \right) / \right. \\ \left. (-9 r_1 r_2^3 r_{22}^2 + 18 r_2^4 r_{22}^2 + 27 r_1 r_2^2 r_{22}^3 - 72 r_2^3 r_{22}^3 - 18 r_1 r_2 r_{22}^4 + 108 r_2^2 r_{22}^4 - 72 r_2 r_{22}^5 + 16 r_{22}^6 + \sqrt{-4 (3 r_2^4 - 12 r_2^3 r_{22} + 18 r_2^2 r_{22}^2 - 12 r_2 r_{22}^3 + 4 r_{22}^4 + 3 r_1 r_2 (r_2^2 - 3 r_2 r_{22} + 2 r_{22}^2))^3 + r_{22}^4 (9 r_1 r_2 (r_2^2 - 3 r_2 r_{22} + 2 r_{22}^2) - 2 (9 r_2^4 - 36 r_2^3 r_{22} + 54 r_2^2 r_{22}^2 - 36 r_2 r_{22}^3 + 8 r_{22}^4))^2})^{1/3}} - 8 \times 2^{2/3} (1 + i \sqrt{3}) (-9 r_1 r_2^3 r_{22}^2 + 18 r_2^4 r_{22}^2 + 27 r_1 r_2^2 r_{22}^3 - 72 r_2^3 r_{22}^3 - 18 r_1 r_2 r_{22}^4 + 108 r_2^2 r_{22}^4 - 72 r_2 r_{22}^5 + 16 r_{22}^6 + \sqrt{-4 (3 r_2^4 - 12 r_2^3 r_{22} + 18 r_2^2 r_{22}^2 - 12 r_2 r_{22}^3 + 4 r_{22}^4 + 3 r_1 r_2 (r_2^2 - 3 r_2 r_{22} + 2 r_{22}^2))^3 + r_{22}^4 (9 r_1 r_2 (r_2^2 - 3 r_2 r_{22} + 2 r_{22}^2) - 2 (9 r_2^4 - 36 r_2^3 r_{22} + 54 r_2^2 r_{22}^2 - 36 r_2 r_{22}^3 + 8 r_{22}^4))^2})^{1/3}} \right) \right\}$$

In[*]:= \$Assumptions =

r12 > 0 && r22 > 0 && r12 + r22 < r2 && Element[r12, Reals] && Element[r22, Reals]

Out[*]:= r12 > 0 && r22 > 0 && r12 + r22 < r2 && r12 ∈ ℝ && r22 ∈ ℝ

In[*]:= Re[solsim]

Out[*]:= {Re[

$$\begin{aligned} r12 \rightarrow & \frac{1}{192 (r2 - r22)} \left(32 (3 r2^2 - 6 r2 r22 + 2 r22^2) + (16 i 2^{1/3} (i + \sqrt{3}) (3 r2^4 - 12 r2^3 r22 + 18 \right. \\ & r2^2 r22^2 - 12 r2 r22^3 + 4 r22^4 + 3 r1 r2 (r2^2 - 3 r2 r22 + 2 r22^2)) \Big) / \\ & \left(-9 r1 r2^3 r22^2 + 18 r2^4 r22^2 + 27 r1 r2^2 r22^3 - 72 r2^3 r22^3 - 18 r1 r2 r22^4 + 108 r2^2 r22^4 - \right. \\ & 72 r2 r22^5 + 16 r22^6 + \sqrt{-4 (3 r2^4 - 12 r2^3 r22 + 18 r2^2 r22^2 - 12 r2 r22^3 + 4 r22^4 +} \\ & 3 r1 r2 (r2^2 - 3 r2 r22 + 2 r22^2))^3 + r22^4 (9 r1 r2 (r2^2 - 3 r2 r22 + 2 r22^2) - \\ & 2 (9 r2^4 - 36 r2^3 r22 + 54 r2^2 r22^2 - 36 r2 r22^3 + 8 r22^4))^2 \Big)^{1/3} - \\ & 8 \times 2^{2/3} (1 + i \sqrt{3}) \left(-9 r1 r2^3 r22^2 + 18 r2^4 r22^2 + 27 r1 r2^2 r22^3 - 72 r2^3 r22^3 - \right. \\ & 18 r1 r2 r22^4 + 108 r2^2 r22^4 - 72 r2 r22^5 + 16 r22^6 + \\ & \sqrt{-4 (3 r2^4 - 12 r2^3 r22 + 18 r2^2 r22^2 - 12 r2 r22^3 + 4 r22^4 +} \\ & 3 r1 r2 (r2^2 - 3 r2 r22 + 2 r22^2))^3 + r22^4 (9 r1 r2 (r2^2 - 3 r2 r22 + 2 r22^2) - \\ & 2 (9 r2^4 - 36 r2^3 r22 + 54 r2^2 r22^2 - 36 r2 r22^3 + 8 r22^4))^2 \Big)^{1/3} \Big) \Big] \Big\} \end{aligned}$$

In[*]:= {r12 → $\frac{1}{192 (r2 - r22)}$

$$\begin{aligned} & \left(32 (3 r2^2 - 6 r2 r22 + 2 r22^2) + (16 i 2^{1/3} (i + \sqrt{3}) (3 r2^3 (r1 + r2) - 3 r2^2 (3 r1 + 4 r2) \right. \\ & r22 + 6 r2 (r1 + 3 r2) r22^2 - 12 r2 r22^3 + 4 r22^4) \Big) / \left(18 r2^4 r22^2 + 16 r22^6 + \right. \\ & 27 r2^2 r22^3 (r1 + 4 r22) - 18 r2 r22^4 (r1 + 4 r22) - 9 r2^3 r22^2 (r1 + 8 r22) + \\ & \sqrt{-4 (3 r2^3 (r1 + r2) - 3 r2^2 (3 r1 + 4 r2) r22 + 6 r2 (r1 + 3 r2) r22^2 -} \\ & 12 r2 r22^3 + 4 r22^4))^3 + r22^4 (9 r1 r2 (r2 - 2 r22) (r2 - r22) - \\ & 2 (3 r2^2 - 6 r2 r22 + 2 r22^2) (3 r2^2 - 6 r2 r22 + 4 r22^2))^2 \Big)^{1/3} - \\ & 8 \times 2^{2/3} (1 + i \sqrt{3}) \left(18 r2^4 r22^2 + 16 r22^6 + 27 r2^2 r22^3 (r1 + 4 r22) - \right. \\ & 18 r2 r22^4 (r1 + 4 r22) - 9 r2^3 r22^2 (r1 + 8 r22) + \\ & \sqrt{-4 (3 r2^3 (r1 + r2) - 3 r2^2 (3 r1 + 4 r2) r22 + 6 r2 (r1 + 3 r2) r22^2 - 12 r2 r22^3 +} \\ & 4 r22^4))^3 + r22^4 (9 r1 r2 (r2 - 2 r22) (r2 - r22) - 2 (3 r2^2 - 6 r2 r22 + \\ & 2 r22^2) (3 r2^2 - 6 r2 r22 + 4 r22^2))^2 \Big)^{1/3} \Big) \Big\} /. ex /. r22 \rightarrow 0.24 \end{aligned}$$

Out[*]:= {r12 → -0.0336525 - 0.106938 i}

In[*]:= sol2 /. ex /. r22 → 0.23

Out[*]:= {{r12 → -0.0828427}, {r12 → 0.482843}, {r12 → -0.0706438}, {r12 → 0.240644},
{r12 → 0.143166}, {r12 → -0.0218773 + 0.0889001 i}, {r12 → -0.0218773 - 0.0889001 i}}

In[*]:= eq = FullSimplify[term1 - term2]

$$\text{Out[*]} = \frac{r1}{4} + r12 - r22 + \frac{(r1 + 4 r12) r22^2}{r1 r2 + 4 r12 (-r12 + r2)} + \frac{r12^2}{-r2 + r22} - \frac{r3}{4}$$

```
In[ ]:= eq3 = FullSimplify[e3]
```

$$\text{Out[]} = \frac{-1 + \frac{2 r_{12}}{r_2 - r_{22}}}{-1 + \frac{2 r_{12}}{r_2 - r_{22}} - \frac{8 r_{12} (r_1 + 2 r_{12}) r_{22}^2}{(r_1 r_2 + 4 r_{12} (-r_{12} + r_2))^2}} == \frac{r_{12}^2}{(r_2 - r_{22})^2 \left(1 + \frac{r_{12}^2}{(r_2 - r_{22})^2} - \frac{2 (r_1 + 4 r_{12}) r_{22}}{r_1 r_2 + 4 r_{12} (-r_{12} + r_2)}\right)}$$

```
In[ ]:= NSolve[{eq == 0 /. ex, eq3 /. ex}, {r12, r22}]
```

```
Out[ ]:= {{r22 -> 7755.25 - 1199.97 I, r12 -> -0.100001 - 1.94884 x 10^-7 I},
  {r22 -> -0.0124558 + 0.106249 I, r12 -> -0.0846366 + 0.00206376 I},
  {r22 -> -0.0124558 - 0.106249 I, r12 -> -0.0846366 - 0.00206376 I},
  {r22 -> 0.183165, r12 -> 0.0615317}, {r22 -> 0.736729, r12 -> 0.7769},
  {r22 -> 0.638789, r12 -> -0.326643},
  {r22 -> 0.28612 - 0.0820165 I, r12 -> 0.0607311 + 0.062323 I},
  {r22 -> 0.28612 + 0.0820165 I, r12 -> 0.0607311 - 0.062323 I},
  {r22 -> 0.28612 + 0.0820165 I, r12 -> 0.0607311 - 0.062323 I},
  {r22 -> 0.0469944 - 0.372019 I, r12 -> 0.468011 + 0.288141 I},
  {r22 -> 0.0469944 + 0.372019 I, r12 -> 0.468011 - 0.288141 I}, {r22 -> 0.2, r12 -> 0.2}}
```

Solutions to plot in R

```
In[ ]:= xx = {r1 -> 0.2, r3 -> 0.1}
```

```
Out[ ]:= {r1 -> 0.2, r3 -> 0.1}
```

```
In[ ]:= x = {r1 -> 0.2, r2 -> 0.7, r3 -> 0.1}
```

```
Out[ ]:= {r1 -> 0.2, r2 -> 0.7, r3 -> 0.1}
```

```
In[ ]:= FindMinimum[
```

```
{(-term1) /. x, term1 == term2 /. x, r12 + r22 < 0.7, r12 > 0, r22 > 0}, {r12, r22}] [[2]]
```

```
Out[ ]:= {r12 -> 0.184831, r22 -> 0.238117}
```

```
In[ ]:= nsol = NSolve[{eq == 0 /. x, eq3 /. x, r12 > 0, r22 > 0, r12 + r22 < r2 /. x}, {r12, r22}]
```

```
Out[ ]:= {{r22 -> 0.647259, r12 -> 0.0329464}, {r22 -> 0.238117, r12 -> 0.184831}}
```

```
In[ ]:= {term1, term2} /. x /. nsol
```

```
Out[ ]:= {{0.0623653, 0.0623653}, {0.160867, 0.160867}}
```

```
In[ ]:= NSolve[{eq == 0 /. {r1 -> 0.2, r2 -> 0.7, r3 -> 0.1},
  eq3 /. {r1 -> 0.2, r2 -> 0.7, r3 -> 0.1}}, {r12, r22}];
```

```
In[ ]:= term1
term2
```

$$\text{Out[]} = \frac{r_1}{4} + r_{12} + \frac{r_{12}^2}{-r_2 + r_{22}}$$

$$\text{Out[]} = r_{22} - \frac{(r_1 + 4 r_{12}) r_{22}^2}{r_1 r_2 + 4 r_{12} (-r_{12} + r_2)} + \frac{r_3}{4}$$


```
In[*]:= v = Range[0.4, 0.9, 0.01]
```

```
f[r2_] := FindMinimum[{- ( -  $\frac{r1}{4} + r12 + \frac{r12^2}{-r2 + r22}$  ) /. {r1 → 0.1},  

 $\frac{r1}{4} + r12 + \frac{r12^2}{-r2 + r22} == r22 - \frac{(r1 + 4 r12) r22^2}{r1 r2 + 4 r12 (-r12 + r2)} + \frac{1 - r1 - r2}{4}$  /. {r1 → 0.1},  

r12 + r22 < r2, r12 > 0, r22 > 0}, {{r12, r2 / 3 /. ex}, {r22, r2 / 3 /. ex}}] [[2]]  

results1 = ({r12, r22} /. Map[f, v]) / v  

Export[  

"/Users/mbofi/Dropbox/CeMSIIS/GitHub/Allocation/optimisation/results1.csv", results1]
```

```
Out[*]:= {0.4, 0.41, 0.42, 0.43, 0.44, 0.45, 0.46, 0.47, 0.48, 0.49, 0.5, 0.51,  

0.52, 0.53, 0.54, 0.55, 0.56, 0.57, 0.58, 0.59, 0.6, 0.61, 0.62, 0.63, 0.64,  

0.65, 0.66, 0.67, 0.68, 0.69, 0.7, 0.71, 0.72, 0.73, 0.74, 0.75, 0.76, 0.77,  

0.78, 0.79, 0.8, 0.81, 0.82, 0.83, 0.84, 0.85, 0.86, 0.87, 0.88, 0.89, 0.9}
```

```
Out[*]:= {{0.5,  $9.57139 \times 10^{-18}$ }, {0.495012, 0.00989618}, {0.490046, 0.0195931},  

{0.485097, 0.0291022}, {0.480161, 0.0384342}, {0.475236, 0.0475985},  

{0.470317, 0.0566038}, {0.465402, 0.0654578}, {0.460488, 0.0741673},  

{0.455574, 0.0827387}, {0.450656, 0.0911774}, {0.445733, 0.0994882},  

{0.440804, 0.107675}, {0.435867, 0.115742}, {0.430922, 0.123692}, {0.425968, 0.131528},  

{0.421005, 0.13925}, {0.416032, 0.146862}, {0.411051, 0.154363}, {0.406061, 0.161754},  

{0.401065, 0.169036}, {0.396062, 0.176208}, {0.391056, 0.183269}, {0.386047, 0.190218},  

{0.381039, 0.197055}, {0.376034, 0.203777}, {0.371035, 0.210383},  

{0.366045, 0.216871}, {0.361068, 0.22324}, {0.356108, 0.229486}, {0.351167, 0.235609},  

{0.346252, 0.241606}, {0.341365, 0.247475}, {0.33651, 0.253214}, {0.331693, 0.258823},  

{0.326917, 0.2643}, {0.322186, 0.269644}, {0.317503, 0.274855}, {0.312874, 0.279931},  

{0.308301, 0.284874}, {0.303787, 0.289682}, {0.299336, 0.294358}, {0.29495, 0.298902},  

{0.290632, 0.303315}, {0.286384, 0.307599}, {0.282207, 0.311756}, {0.278103, 0.315788},  

{0.274074, 0.319697}, {0.27012, 0.323485}, {0.266241, 0.327157}, {0.262438, 0.330714}}
```

```
Out[*]:= /Users/mbofi/Dropbox/CeMSIIS/GitHub/Allocation/optimisation/results1.csv
```

```
In[ ]:= v = Range[0.2, 0.7, 0.01]
```

```
f[r2_] := FindMinimum[{- ( -  $\frac{r1}{4} + r12 + \frac{r12^2}{-r2 + r22}$  ) /. {r1 → 0.3},  

 $\frac{r1}{4} + r12 + \frac{r12^2}{-r2 + r22} == r22 - \frac{(r1 + 4 r12) r22^2}{r1 r2 + 4 r12 (-r12 + r2)} + \frac{1 - r1 - r2}{4}$  /. {r1 → 0.3},  

r12 + r22 < r2, r12 > 0, r22 > 0}, {{r12, r2 / 3 /. ex}, {r22, r2 / 3 /. ex}}] [[2]]  

results2 = ({r12, r22} /. Map[f, v]) / v  

Export["/Users/mbofi/Dropbox/CeMSIIS/GitHub/Allocation/optimisation/results2.csv",  

results2]
```

```
Out[ ]:= {0.2, 0.21, 0.22, 0.23, 0.24, 0.25, 0.26, 0.27, 0.28, 0.29, 0.3, 0.31,  

0.32, 0.33, 0.34, 0.35, 0.36, 0.37, 0.38, 0.39, 0.4, 0.41, 0.42, 0.43, 0.44,  

0.45, 0.46, 0.47, 0.48, 0.49, 0.5, 0.51, 0.52, 0.53, 0.54, 0.55, 0.56, 0.57,  

0.58, 0.59, 0.6, 0.61, 0.62, 0.63, 0.64, 0.65, 0.66, 0.67, 0.68, 0.69, 0.7}
```

```
Out[ ]:= {{0.5,  $9.4495 \times 10^{-18}$ }, {0.490186, 0.019471}, {0.480706, 0.0379681}, {0.47151, 0.0556027},  

{0.462555, 0.0724689}, {0.453806, 0.0886466}, {0.445229, 0.104204},  

{0.436797, 0.119199}, {0.428487, 0.133681}, {0.420277, 0.147693}, {0.412149, 0.161269},  

{0.404088, 0.17444}, {0.396082, 0.187229}, {0.388118, 0.199657}, {0.38019, 0.211738},  

{0.372291, 0.223484}, {0.364417, 0.234902}, {0.356568, 0.245995}, {0.348744, 0.256764},  

{0.34095, 0.267208}, {0.333192, 0.277321}, {0.325478, 0.287098}, {0.317819, 0.296532},  

{0.310229, 0.305614}, {0.302721, 0.314336}, {0.295311, 0.322692}, {0.288015, 0.330677},  

{0.280849, 0.338288}, {0.273828, 0.345522}, {0.266967, 0.352384}, {0.260278, 0.358877},  

{0.253771, 0.36501}, {0.247456, 0.370792}, {0.241337, 0.376236}, {0.235419, 0.381356},  

{0.229704, 0.386167}, {0.224191, 0.390686}, {0.218878, 0.394928}, {0.213763, 0.398912},  

{0.208841, 0.402652}, {0.204106, 0.406166}, {0.199552, 0.409468}, {0.195174, 0.412574},  

{0.190965, 0.415497}, {0.186917, 0.41825}, {0.183025, 0.420846}, {0.17928, 0.423295},  

{0.175676, 0.425609}, {0.172208, 0.427797}, {0.168868, 0.429868}, {0.16565, 0.43183}}
```

```
Out[ ]:= /Users/mbofi/Dropbox/CeMSIIS/GitHub/Allocation/optimisation/results2.csv
```

```
In[ ]:= v = Range[0.1, 0.6, 0.01]
```

```
f[r2_] := FindMinimum[{- (r1/4 + r12 + r12^2/(-r2 + r22)) /. {r1 -> 0.4},
  r1/4 + r12 + r12^2/(-r2 + r22) == r22 - (r1 + 4 r12) r22^2/(r1 r2 + 4 r12 (-r12 + r2)) + (1 - r1 - r2)/4 /. {r1 -> 0.4},
  r12 + r22 < r2, r12 > 0, r22 > 0}, {{r12, r2/3 /. ex}, {r22, r2/3 /. ex}}] [[2]]
```

```
results3 = ({r12, r22} /. Map[f, v]) / v
```

```
Export[
```

```
"/Users/mbofi/Dropbox/CeMSIIS/GitHub/Allocation/optimisation/results3.csv", results3]
```

```
Out[ ]:= {0.1, 0.11, 0.12, 0.13, 0.14, 0.15, 0.16, 0.17, 0.18, 0.19, 0.2, 0.21,
  0.22, 0.23, 0.24, 0.25, 0.26, 0.27, 0.28, 0.29, 0.3, 0.31, 0.32, 0.33, 0.34,
  0.35, 0.36, 0.37, 0.38, 0.39, 0.4, 0.41, 0.42, 0.43, 0.44, 0.45, 0.46, 0.47,
  0.48, 0.49, 0.5, 0.51, 0.52, 0.53, 0.54, 0.55, 0.56, 0.57, 0.58, 0.59, 0.6}
```

```
Out[ ]:= {{0.5, 0.}, {0.48098, 0.0377298}, {0.463606, 0.0715795}, {0.447502, 0.102335},
  {0.432383, 0.130579}, {0.418029, 0.156753}, {0.404266, 0.181198}, {0.390951, 0.204176},
  {0.377971, 0.225889}, {0.365227, 0.24649}, {0.352641, 0.266093}, {0.34015, 0.284773},
  {0.327707, 0.302568}, {0.315285, 0.319486}, {0.302877, 0.335501}, {0.290505, 0.350562},
  {0.278221, 0.364598}, {0.266103, 0.377533}, {0.254253, 0.389306}, {0.242782, 0.399886},
  {0.231791, 0.409285}, {0.221362, 0.417557}, {0.211546, 0.42479}, {0.202362, 0.431094},
  {0.193807, 0.436583}, {0.185857, 0.441369}, {0.178476, 0.445556}, {0.171626, 0.449232},
  {0.165262, 0.452475}, {0.159343, 0.45535}, {0.153829, 0.457912}, {0.148684, 0.460205},
  {0.143875, 0.462267}, {0.13937, 0.464131}, {0.135143, 0.465822}, {0.131169, 0.467362},
  {0.127427, 0.468771}, {0.123897, 0.470064}, {0.120562, 0.471255}, {0.117405, 0.472354},
  {0.114413, 0.473373}, {0.111573, 0.474319}, {0.108874, 0.475201}, {0.106305, 0.476023},
  {0.103858, 0.476793}, {0.101522, 0.477514}, {0.099292, 0.478192},
  {0.0971595, 0.47883}, {0.0951185, 0.479432}, {0.0931631, 0.48}, {0.091288, 0.480537}}
```

```
Out[ ]:= /Users/mbofi/Dropbox/CeMSIIS/GitHub/Allocation/optimisation/results3.csv
```

```
In[ ]:= v = Range[0.01, 0.49, 0.002]
```

```
f[r2_] := FindMinimum[{- (r1/4 + r12 + r12^2/(-r2 + r22)) /. {r1 -> 0.49},
  r1/4 + r12 + r12^2/(-r2 + r22) == r22 - (r1 + 4 r12) r22^2/(r1 r2 + 4 r12 (-r12 + r2)) + (1 - r1 - r2)/4 /. {r1 -> 0.49},
  r12 + r22 < r2, r12 > 0, r22 > 0}, {{r12, r2/20 /. ex}, {r22, r2/2 /. ex}}] [[2]]
```

```
results4 = ({r12, r22} /. Map[f, v]) / v
```

```
Export[
```

```
"/Users/mbofi/Dropbox/CeMSIIS/GitHub/Allocation/optimisation/results4.csv", results4]
```

```
Out[ ]= {0.01, 0.012, 0.014, 0.016, 0.018, 0.02, 0.022, 0.024, 0.026, 0.028, 0.03, 0.032, 0.034,
0.036, 0.038, 0.04, 0.042, 0.044, 0.046, 0.048, 0.05, 0.052, 0.054, 0.056, 0.058,
0.06, 0.062, 0.064, 0.066, 0.068, 0.07, 0.072, 0.074, 0.076, 0.078, 0.08, 0.082,
0.084, 0.086, 0.088, 0.09, 0.092, 0.094, 0.096, 0.098, 0.1, 0.102, 0.104, 0.106,
0.108, 0.11, 0.112, 0.114, 0.116, 0.118, 0.12, 0.122, 0.124, 0.126, 0.128, 0.13,
0.132, 0.134, 0.136, 0.138, 0.14, 0.142, 0.144, 0.146, 0.148, 0.15, 0.152, 0.154,
0.156, 0.158, 0.16, 0.162, 0.164, 0.166, 0.168, 0.17, 0.172, 0.174, 0.176, 0.178,
0.18, 0.182, 0.184, 0.186, 0.188, 0.19, 0.192, 0.194, 0.196, 0.198, 0.2, 0.202,
0.204, 0.206, 0.208, 0.21, 0.212, 0.214, 0.216, 0.218, 0.22, 0.222, 0.224, 0.226,
0.228, 0.23, 0.232, 0.234, 0.236, 0.238, 0.24, 0.242, 0.244, 0.246, 0.248, 0.25,
0.252, 0.254, 0.256, 0.258, 0.26, 0.262, 0.264, 0.266, 0.268, 0.27, 0.272, 0.274,
0.276, 0.278, 0.28, 0.282, 0.284, 0.286, 0.288, 0.29, 0.292, 0.294, 0.296, 0.298,
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