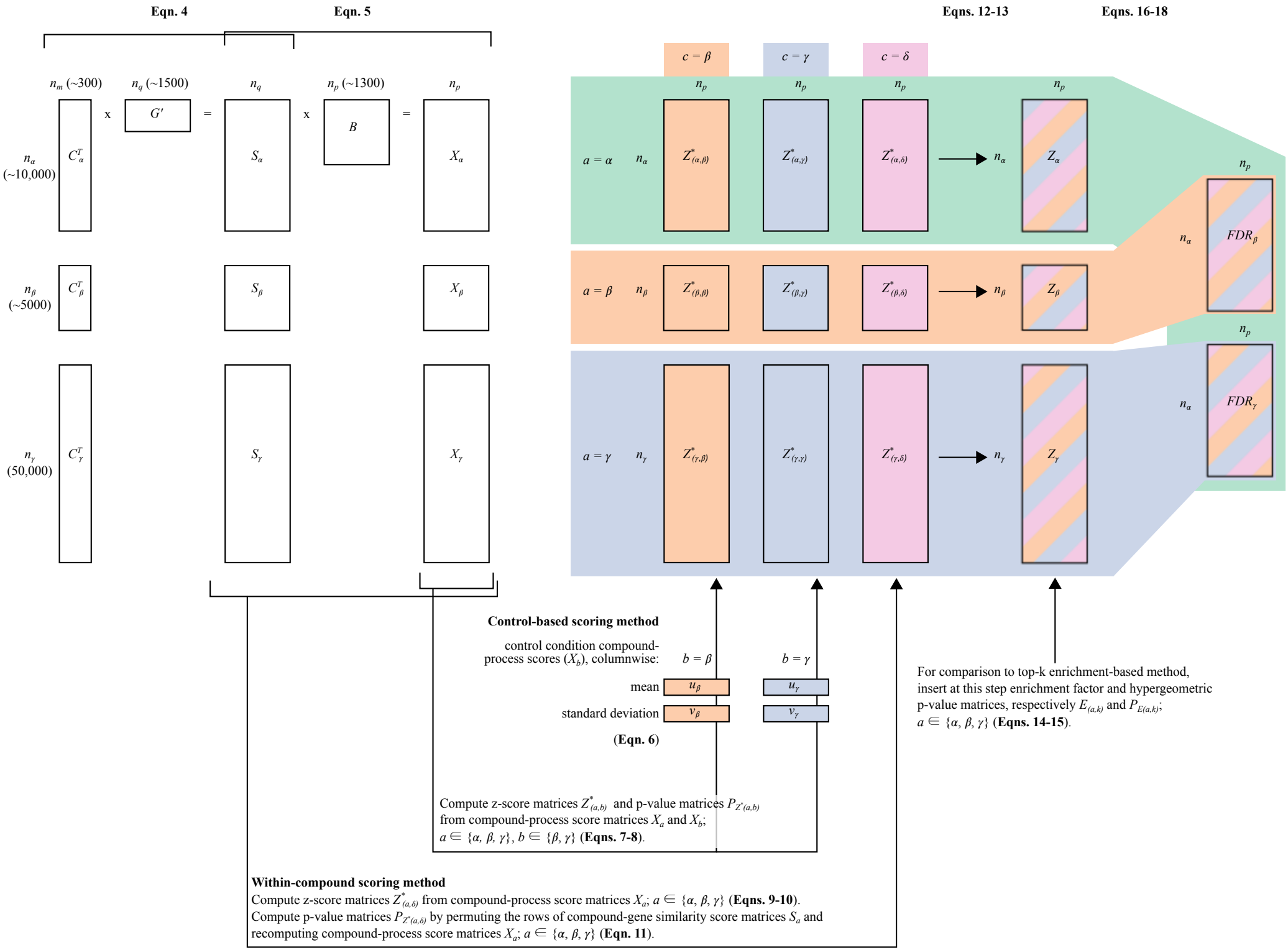
Eqn. 4
Eqn. 5
Eqns. 12-13
Eqns. 16-18
n_m (~300)
n_q (~1500)
n_q
n_p (~1300)
n_p
G'
B
n_α (~10,000)
n_β (~5000)
n_γ (50,000)
C^T_α
C^T_β
C^T_γ
S_α
S_β
S_γ
X_α
X_β
X_γ
$c = \beta$
$c = \gamma$
$c = \delta$
$a = \alpha$
$a = \beta$
$a = \gamma$
$Z^*_{(\alpha,\beta)}$
$Z^*_{(\alpha,\gamma)}$
$Z^*_{(\alpha,\delta)}$
$Z^*_{(\beta,\beta)}$
$Z^*_{(\beta,\gamma)}$
$Z^*_{(\beta,\delta)}$
$Z^*_{(\gamma,\beta)}$
$Z^*_{(\gamma,\gamma)}$
$Z^*_{(\gamma,\delta)}$
Z_α
Z_β
Z_γ
FDR_β
FDR_γ
Control-based scoring method
control condition compound-process scores (X_b), columnwise:
$b = \beta$
$b = \gamma$
mean
standard deviation
u_β
v_β
u_γ
v_γ
(Eqn. 6)
For comparison to top-k enrichment-based method, insert at this step enrichment factor and hypergeometric p-value matrices, respectively $E_{(a,k)}$ and $P_{E(a,k)}$; $a \in \{\alpha, \beta, \gamma\}$ (**Eqns. 14-15**).
Compute z-score matrices $Z^*_{(a,b)}$ and p-value matrices $P_{Z^*(a,b)}$ from compound-process score matrices X_a and X_b; $a \in \{\alpha, \beta, \gamma\}$, $b \in \{\beta, \gamma\}$ (**Eqns. 7-8**).
Within-compound scoring method
Compute z-score matrices $Z^*_{(a,\delta)}$ from compound-process score matrices X_a; $a \in \{\alpha, \beta, \gamma\}$ (**Eqns. 9-10**).
Compute p-value matrices $P_{Z^*(a,\delta)}$ by permuting the rows of compound-gene similarity score matrices S_a and recomputing compound-process score matrices X_a; $a \in \{\alpha, \beta, \gamma\}$ (**Eqn. 11**).