**表S1模型在DREAM4 InSilico Size10数据集上推理不同子网络对应的参数**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **MMFGRN** | | | | |
| **DREAM4 InSilico Size10** | **M1** | | **M2 (Score3)** | **M3 (Score4)** |
| **Local-in** | **Local-out** |
| **Network 1** | p+=3  boosting\_type=‘dart’  max\_depth=4  num\_leaves=50  learning\_rate=0.009  min\_child\_samples=17  min\_child\_weight=0.001  colsample\_bytree=0.9  importance\_type= ‘gain’ | p-=3  boosting\_type=‘dart’  max\_depth=4  num\_leaves=50  learning\_rate=0.009  min\_child\_samples=17  min\_child\_weight=0.001  colsample\_bytree=0.9  importance\_type= ‘gain’ | boosting\_type=‘goss’  max\_depth=4  num\_leaves=30  learning\_rate=0.01  min\_child\_samples=1  min\_child\_weight=0.001  colsample\_bytree=0.8  importance\_type= ‘gain’ | c=0.02  max\_depth=5  learning\_rate=0.01  importance\_type='weight' |
| **Network 2** | p+=2  boosting\_type=‘dart’  max\_depth=2  num\_leaves=50  learning\_rate=0.009  min\_child\_samples=20  min\_child\_weight=0.001  colsample\_bytree=0.8  importance\_type= ‘gain’ | p-=2  boosting\_type=‘dart’  max\_depth=2  num\_leaves=50  learning\_rate=0.009  min\_child\_samples=20  min\_child\_weight=0.001  colsample\_bytree=0.8  importance\_type= ‘gain’ | boosting\_type=‘goss’  max\_depth=4  num\_leaves=30  learning\_rate=0.01  min\_child\_samples=1  min\_child\_weight=0.001  colsample\_bytree=0.5  importance\_type= ‘gain’ | c=0.01  max\_depth=5  learning\_rate=0.01  importance\_type='weight' |
| **Network 3** | p+=3  boosting\_type=‘dart’  max\_depth=2  num\_leaves=50  learning\_rate=0.009  min\_child\_samples=17  min\_child\_weight=0.001  colsample\_bytree=0.8  importance\_type= ‘gain’ | p-=3  boosting\_type=‘dart’  max\_depth=2  num\_leaves=50  learning\_rate=0.009  min\_child\_samples=17  min\_child\_weight=0.001  colsample\_bytree=0.8  importance\_type= ‘gain’ | boosting\_type=‘goss’  max\_depth=4  num\_leaves=30  learning\_rate=0.01  min\_child\_samples=1  min\_child\_weight=0.001  colsample\_bytree=0.2  importance\_type= ‘gain’ | c=0.01  max\_depth=5  learning\_rate=0.01  importance\_type='weight' |
| **Network 4** | p+=3  boosting\_type=‘dart’  max\_depth=2  num\_leaves=50  learning\_rate=0.009  min\_child\_samples=20  min\_child\_weight=0.001  colsample\_bytree=0.5  importance\_type= ‘gain’ | p-=3  boosting\_type=‘dart’  max\_depth=2  num\_leaves=50  learning\_rate=0.009  min\_child\_samples=20  min\_child\_weight=0.001  colsample\_bytree=0.5  importance\_type= ‘gain’ | boosting\_type=‘goss’  max\_depth=4  num\_leaves=30  learning\_rate=0.01  min\_child\_samples=4  min\_child\_weight=0.001  colsample\_bytree=0.5  importance\_type= ‘gain’ | c=0.01  max\_depth=5  learning\_rate=0.2  importance\_type='weight' |
| **Network 5** | p+=2  boosting\_type=‘dart’  max\_depth=2  num\_leaves=50  learning\_rate=0.009  min\_child\_samples=17  min\_child\_weight=0.001  colsample\_bytree=0.6  importance\_type= ‘gain’ | p-=2  boosting\_type=‘dart’  max\_depth=2  num\_leaves=50  learning\_rate=0.009  min\_child\_samples=17  min\_child\_weight=0.001  colsample\_bytree=0.6  importance\_type= ‘gain’ | boosting\_type=‘goss’  max\_depth=7  num\_leaves=30  learning\_rate=0.01  min\_child\_samples=1  min\_child\_weight=0.001  colsample\_bytree=0.6  importance\_type= ‘gain’ | c=0.01  max\_depth=5  learning\_rate=0.2  importance\_type='weight' |

*Note*: p-: previous p time points; p+: following p time points; c: decay rate

**表S2模型在DREAM4 InSilico Size100数据集上推理不同子网络对应的参数**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **MMFGRN** | | | | |
| **DREAM4 InSilico Size100** | **M1** | | **M2 (Score3)** | **M3 (Score4)** |
| Local-in (Score1) | Local-out (Score2) |
| **Network 1** | p+=2  boosting\_type=‘dart’  max\_depth=7  num\_leaves=50  learning\_rate=0.009  min\_child\_samples=20  min\_child\_weight=0.001  colsample\_bytree=0.8  importance\_type= ‘gain’ | p-=2  boosting\_type=‘dart’  max\_depth=7  num\_leaves=50  learning\_rate=0.009  min\_child\_samples=20  min\_child\_weight=0.001  colsample\_bytree=0.2  importance\_type= ‘gain’ | boosting\_type=‘goss’  max\_depth=4  num\_leaves=30  learning\_rate=0.01  min\_child\_samples=1  min\_child\_weight=0.001  colsample\_bytree=0.8  importance\_type= ‘gain’ | c=0.01  max\_depth=4  learning\_rate=0.01  importance\_type='weight' |
| **Network 2** | p+=2  boosting\_type=‘dart’  max\_depth=4  num\_leaves=50  learning\_rate=0.009  min\_child\_samples=20  min\_child\_weight=0.001  colsample\_bytree=0.8  importance\_type= ‘gain’ | p-=2  boosting\_type=‘dart’  max\_depth=4  num\_leaves=50  learning\_rate=0.009  min\_child\_samples=20  min\_child\_weight=0.001  colsample\_bytree=0.1  importance\_type= ‘gain’ | boosting\_type=‘goss’  max\_depth=4  num\_leaves=30  learning\_rate=0.01  min\_child\_samples=1  min\_child\_weight=0.001  colsample\_bytree=1  importance\_type= ‘gain’ | c=0.01  max\_depth=4  learning\_rate=0.01  importance\_type='weight' |
| **Network 3** | p+=2  boosting\_type=‘dart’  max\_depth=4  num\_leaves=50  learning\_rate=0.009  min\_child\_samples=20  min\_child\_weight=0.001  colsample\_bytree=0.8  importance\_type= ‘gain’ | p-=2  boosting\_type=‘dart’  max\_depth=4  num\_leaves=50  learning\_rate=0.009  min\_child\_samples=20  min\_child\_weight=0.001  colsample\_bytree=0.1  importance\_type= ‘gain’ | boosting\_type=‘goss’  max\_depth=4  num\_leaves=30  learning\_rate=0.01  min\_child\_samples=1  min\_child\_weight=0.001  colsample\_bytree=0.8  importance\_type= ‘gain’ | c=0.01  max\_depth=4  learning\_rate=0.01  importance\_type='weight' |
| **Network 4** | p+=2  boosting\_type=‘dart’  max\_depth=3  num\_leaves=50  learning\_rate=0.009  min\_child\_samples=20  min\_child\_weight=0.001  colsample\_bytree=1  importance\_type= ‘gain’ | p-=2  boosting\_type=‘dart’  max\_depth=3  num\_leaves=50  learning\_rate=0.009  min\_child\_samples=20  min\_child\_weight=0.001  colsample\_bytree=0.1  importance\_type= ‘gain’ | boosting\_type=‘goss’  max\_depth=4  num\_leaves=30  learning\_rate=0.01  min\_child\_samples=1  min\_child\_weight=0.001  colsample\_bytree=0.5  importance\_type= ‘gain’ | c=0.01  max\_depth=4  learning\_rate=0.01  importance\_type='weight' |
| **Network 5** | p+=2  boosting\_type=‘dart’  max\_depth=3  num\_leaves=50  learning\_rate=0.009  min\_child\_samples=30  min\_child\_weight=0.001  colsample\_bytree=1  importance\_type= ‘gain’ | p-=2  boosting\_type=‘dart’  max\_depth=3  num\_leaves=50  learning\_rate=0.009  min\_child\_samples=30  min\_child\_weight=0.001  colsample\_bytree=0.1  importance\_type= ‘gain’ | boosting\_type=‘goss’  max\_depth=7  num\_leaves=30  learning\_rate=0.01  min\_child\_samples=1  min\_child\_weight=0.001  colsample\_bytree=0.5  importance\_type= ‘gain’ | c=0.01  max\_depth=5  learning\_rate=0.2  importance\_type='weight' |

*Note*: p-: previous p time points; p+: following p time points; c: decay rate