

```
In[733]:= ABMInputs1600 = Import[
  "/Users/thorsilver/Downloads/ABM outputs1/LPtau1600runs_GEMSA_inputs.csv"];

ABMOutputs1600 = Import[
  "/Users/thorsilver/Downloads/ABM outputs1/LPtau1600runs GEMSA outputs.csv"];
```

```
In[735]:= ABMOutputs1600 = Function[x, x/1000] /@ ABMOutputs1600;
ABMAssoc1600 = AssociationThread[ABMInputs1600 → Flatten[ABMOutputs1600]];
ABMnewData1600 = Dataset[ABMAssoc1600];
ABMNormal1600 = Normal[ABMAssoc1600];
ABMNormalRandom = RandomSample[ABMNormal1600];
ABMtrain1600 = TakeDrop[ABMNormal1600, 1280];
ABMtest1600 = ABMtrain1600[[2]];
ABMtraining1600 = ABMtrain1600[[1]];
trainDevSplit1600 = TakeDrop[ABMtraining1600, 1024];
finalTrain1600 = trainDevSplit1600[[1]];
finalDev1600 = trainDevSplit1600[[2]];
finaltest1600 = ABMtest1600;
```

```
In[747]:= Length[finalDev1600]
Length[finalTrain1600]
Length[finaltest1600]
```

Out[747]= 256


Out[748]= 1024

Out[749]= 320

```
In[750]:= pRFv1600 = Predict[finalTrain1600, Method → "RandomForest"]
```

Out[750]= PredictorFunction[ Input type: Mixed (number: 10)
Method: RandomForest]

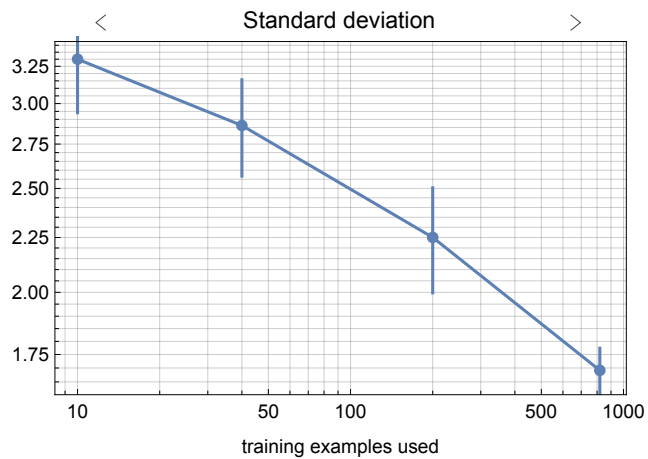
```
In[751]:= pmRFv1600 = PredictorMeasurements[pRFv1600, finaltest1600]
PredictorInformation[pRFv1600]
pmRFv1600["ComparisonPlot"]
pmRFv1600["ResidualPlot"]
```

Out[751]= PredictorMeasurementsObject[ Predictor: RandomForest
Number of test examples: 320]

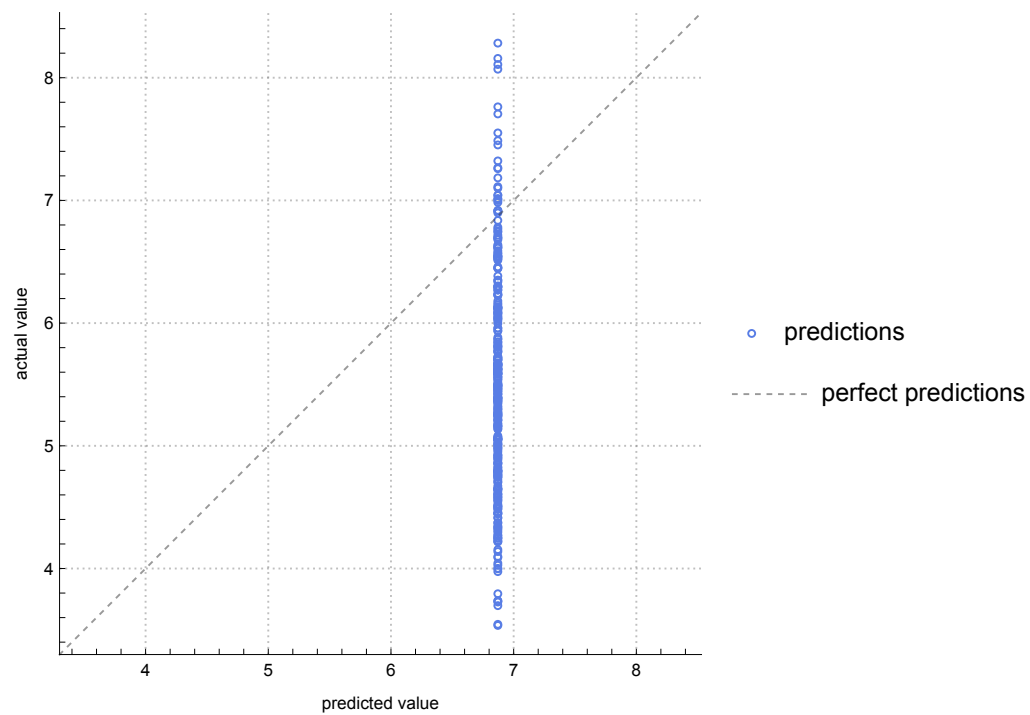
Predictor information

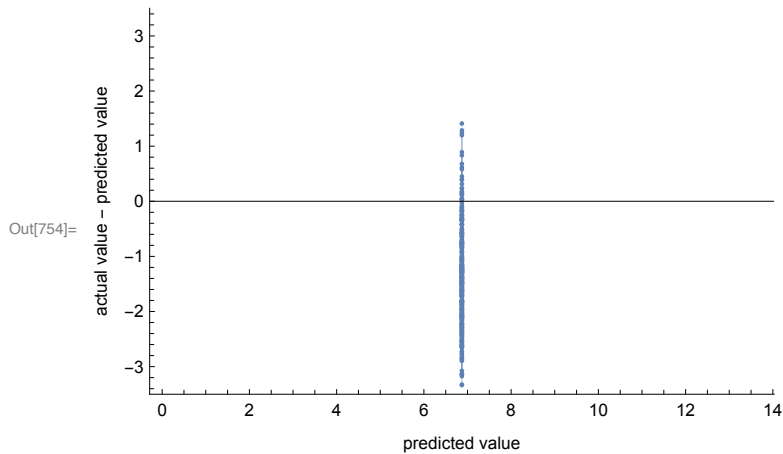
Data type	Mixed (number: 10)
Standard deviation	1.69 ± 0.082
Method	RandomForest
Single evaluation time	3.47 ms/example
Batch evaluation speed	44. examples/ms
Loss	1.88 ± 0.042
Model memory	293. kB
Training examples used	1024 examples
Training time	666. ms

Out[752]=




Out[753]=





```
In[755]:= pXGTV1600 = Predict[finalTrain1600, Method -> "GradientBoostedTrees"]
pmXGTV1600 = PredictorMeasurements[pXGTV1600, finaltest1600]
PredictorInformation[pXGTV1600]
pmXGTV1600["ComparisonPlot"]
pmXGTV1600["ResidualPlot"]
```

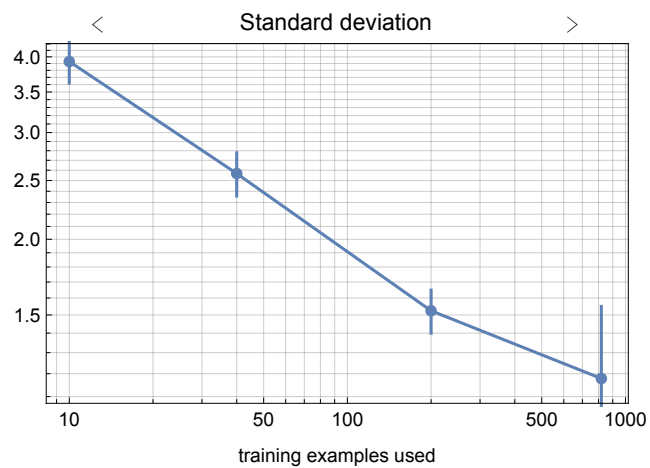
Out[755]= PredictorFunction [  Input type: Mixed (number: 10)
Method: GradientBoostedTrees]

Out[756]= PredictorMeasurementsObject [  Predictor: GradientBoostedTrees
Number of test examples: 320]

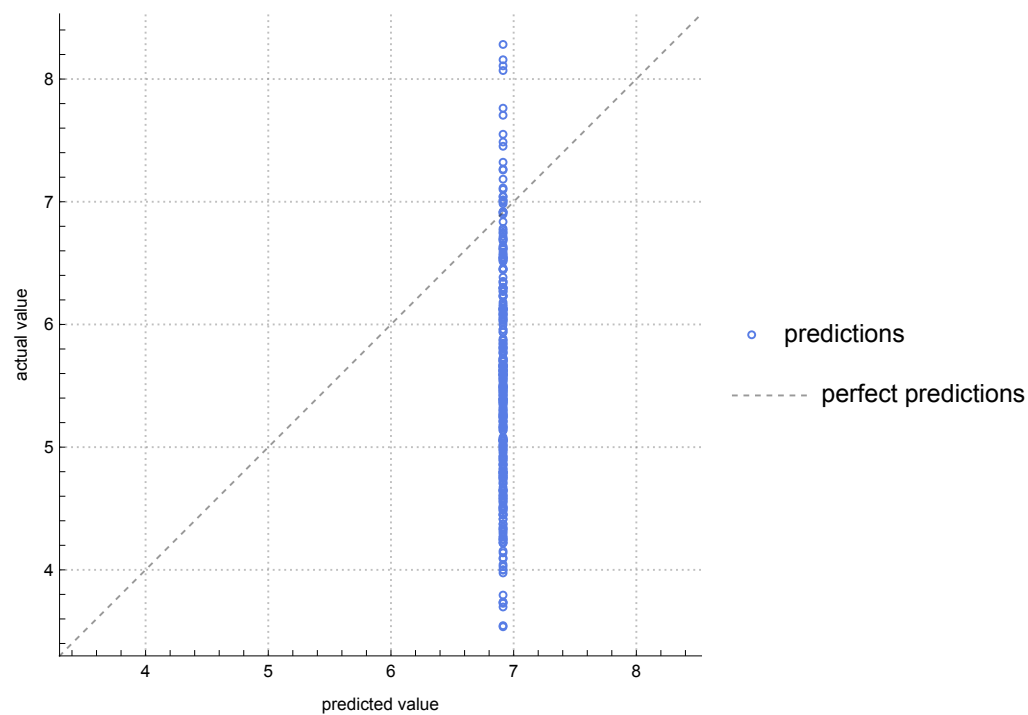
Predictor information

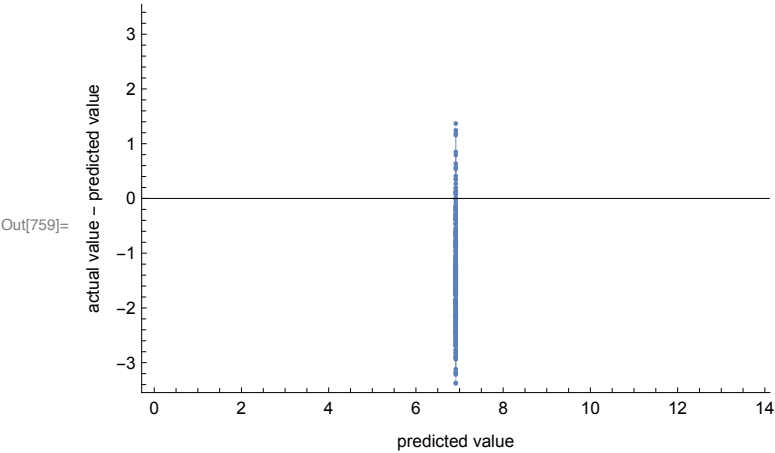
Data type	Mixed (number: 10)
Standard deviation	1.18 ± 0.37
Method	GradientBoostedTrees
Single evaluation time	3.62 ms/example
Batch evaluation speed	49. examples/ms
Loss	6.01 ± 1.4
Model memory	451. kB
Training examples used	1024 examples
Training time	2.57 s

Out[757]=



Out[758]=





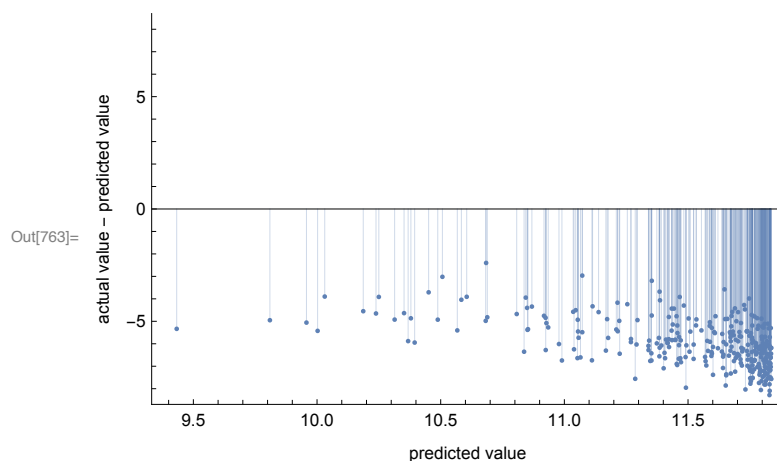
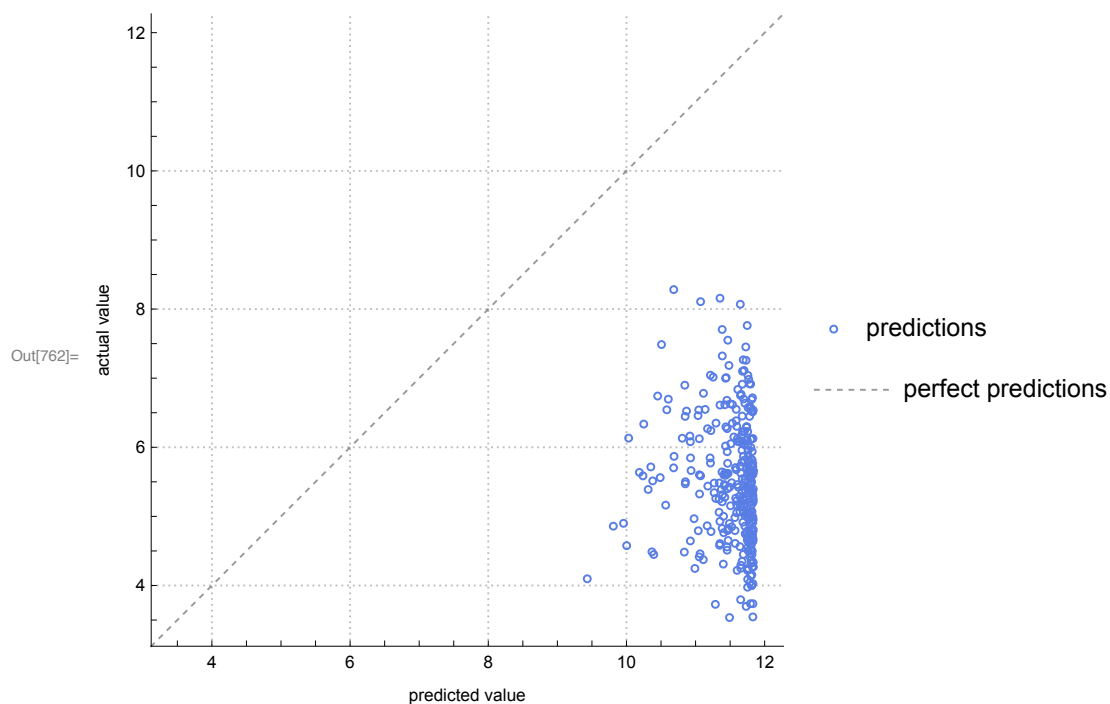
```

In[760]:= pGPEv1600 = Predict[finalTrain1600, Method → "GaussianProcess"]
pmGPEv1600 = PredictorMeasurements[pGPEv1600, finaltest1600]
pmGPEv1600["ComparisonPlot"]
pmGPEv1600["ResidualPlot"]

```

Out[760]= PredictorFunction[ Input type: Mixed (number: 10)
Method: GaussianProcess]


Out[761]= PredictorMeasurementsObject[ Predictor: GaussianProcess
Number of test examples: 320]




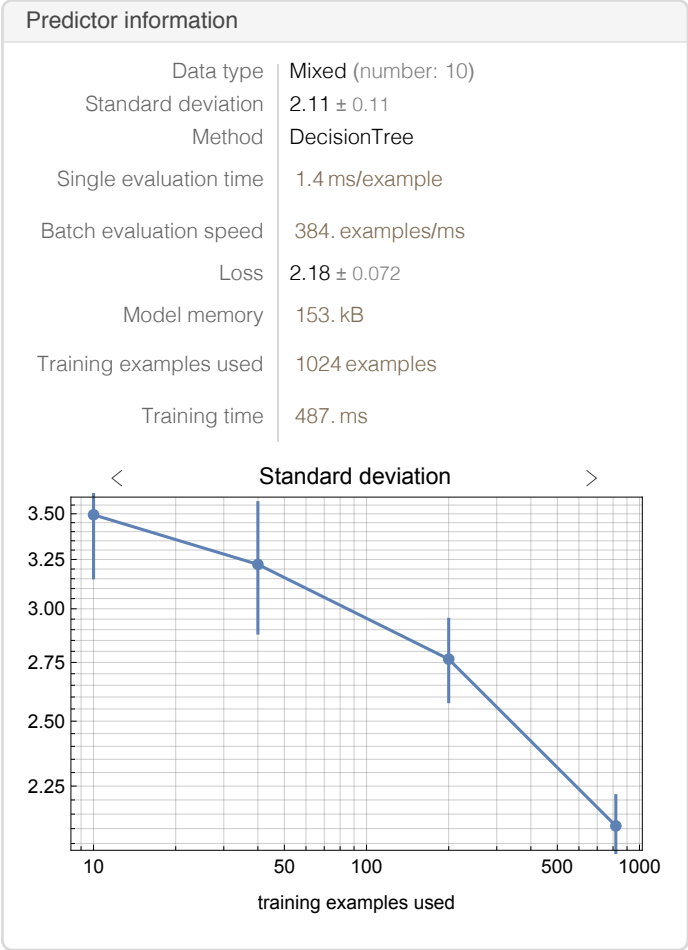
```

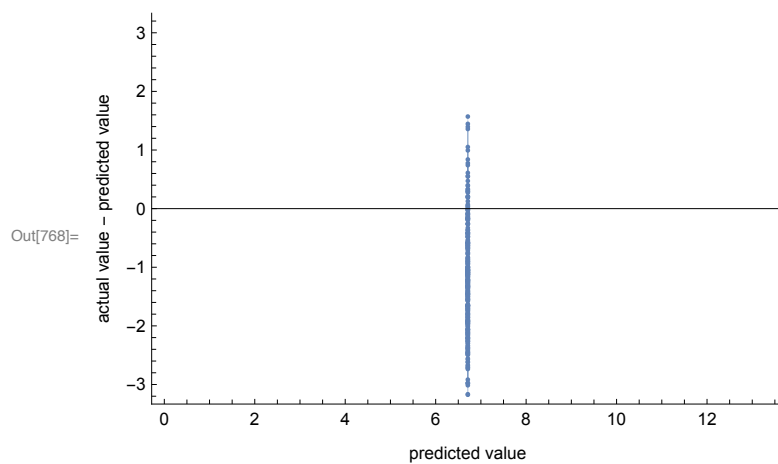
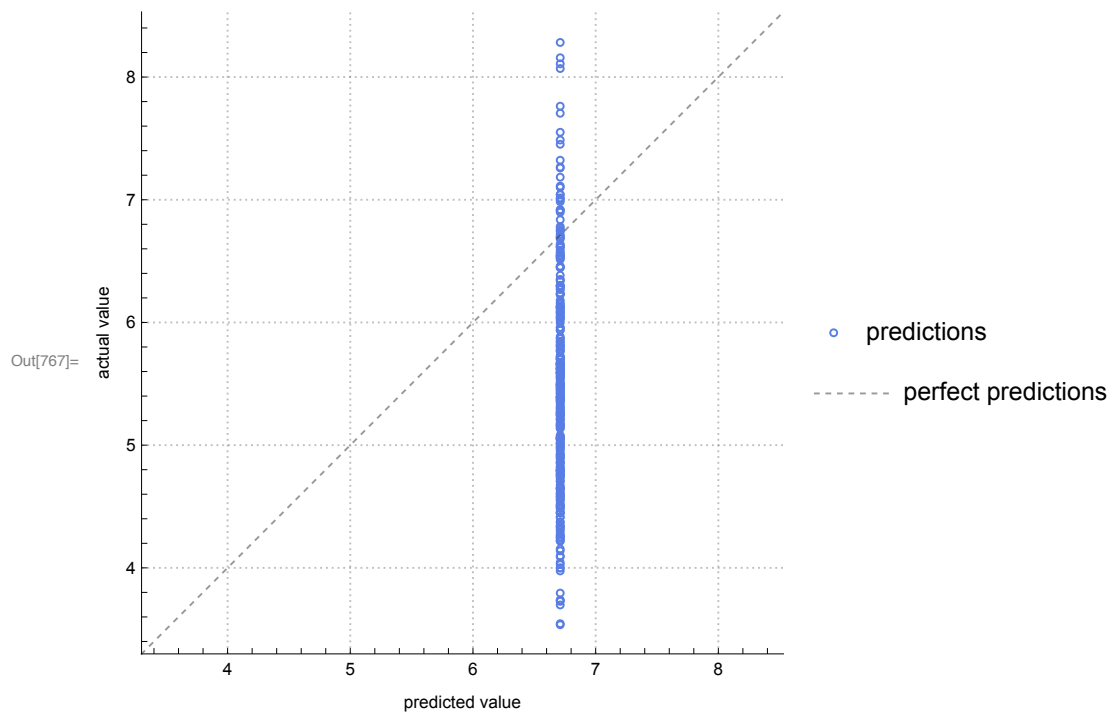
In[764]:= pDTv1600 = Predict[finalTrain1600, Method → "DecisionTree"]
pmDTv1600 = PredictorMeasurements[pDTv1600, finaltest1600]
PredictorInformation[pDTv1600]
pmDTv1600["ComparisonPlot"]
pmDTv1600["ResidualPlot"]

```

Out[764]= PredictorFunction [ Input type: Mixed (number: 10)
Method: DecisionTree]

Out[765]= PredictorMeasurementsObject [ Predictor: DecisionTree
Number of test examples: 320]





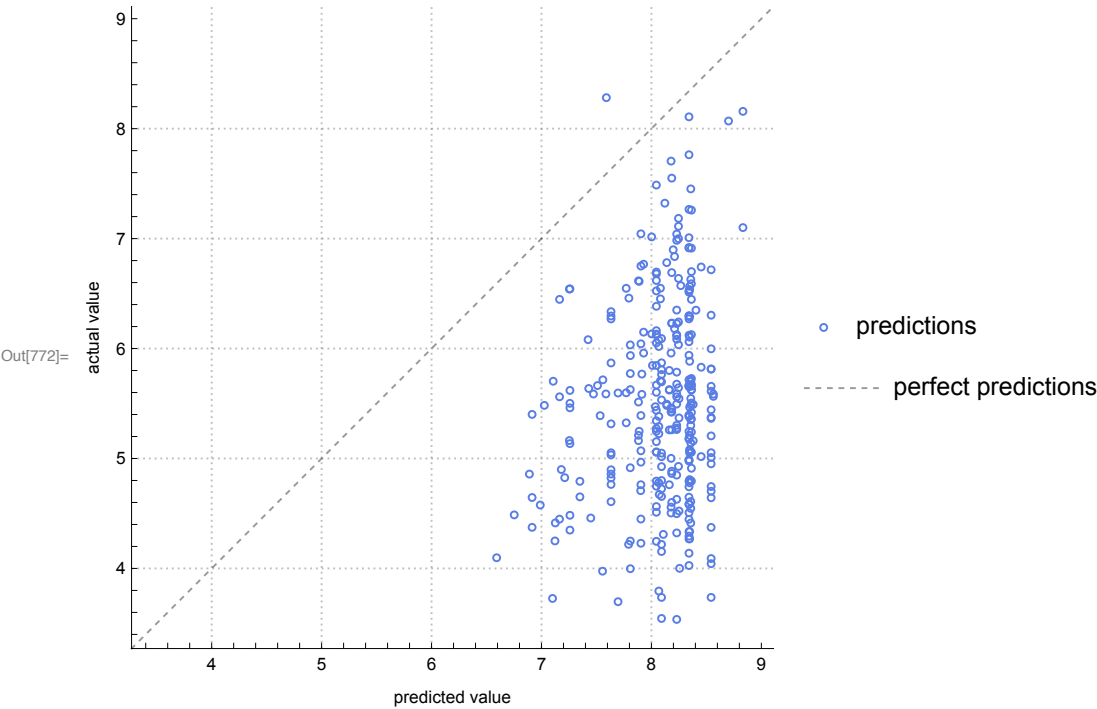
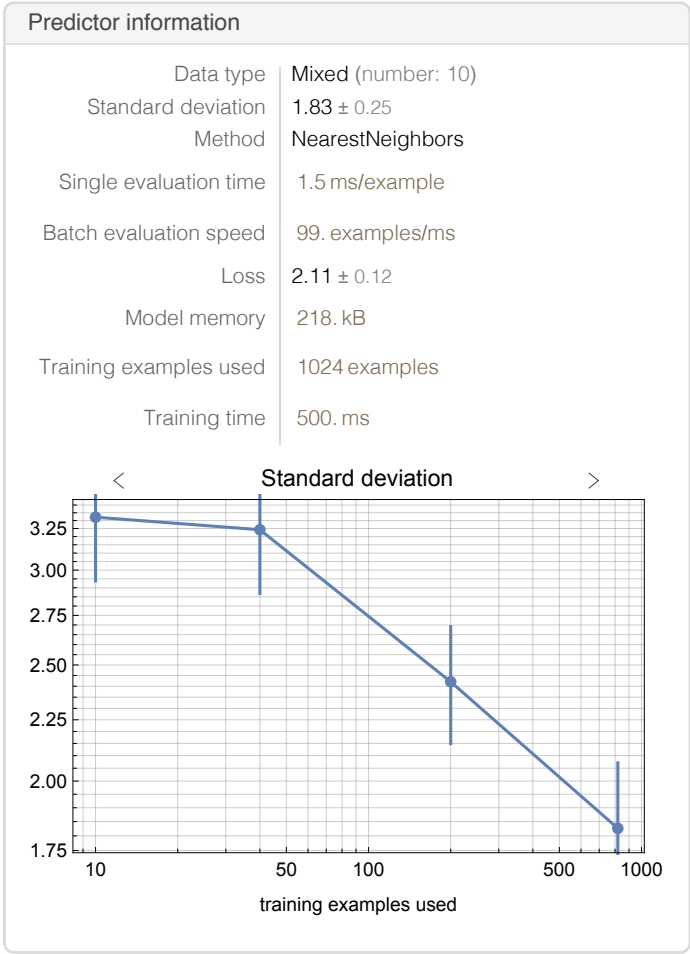
```
In[769]:= pNearestv1600 = Predict[finalTrain1600, Method → "NearestNeighbors"]
pmNearestv1600 = PredictorMeasurements[pNearestv1600, finaltest1600]
PredictorInformation[pNearestv1600]
pmNearestv1600["ComparisonPlot"]
pmNearestv1600["ResidualPlot"]
```

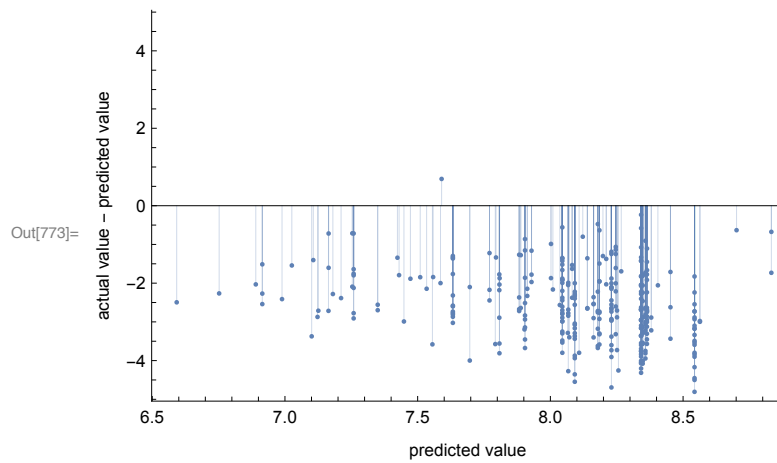
Out[769]=

Input type: Mixed (number: 10)
 Method: NearestNeighbors


Out[770]=


Predictor: NearestNeighbors
 Number of test examples: 320

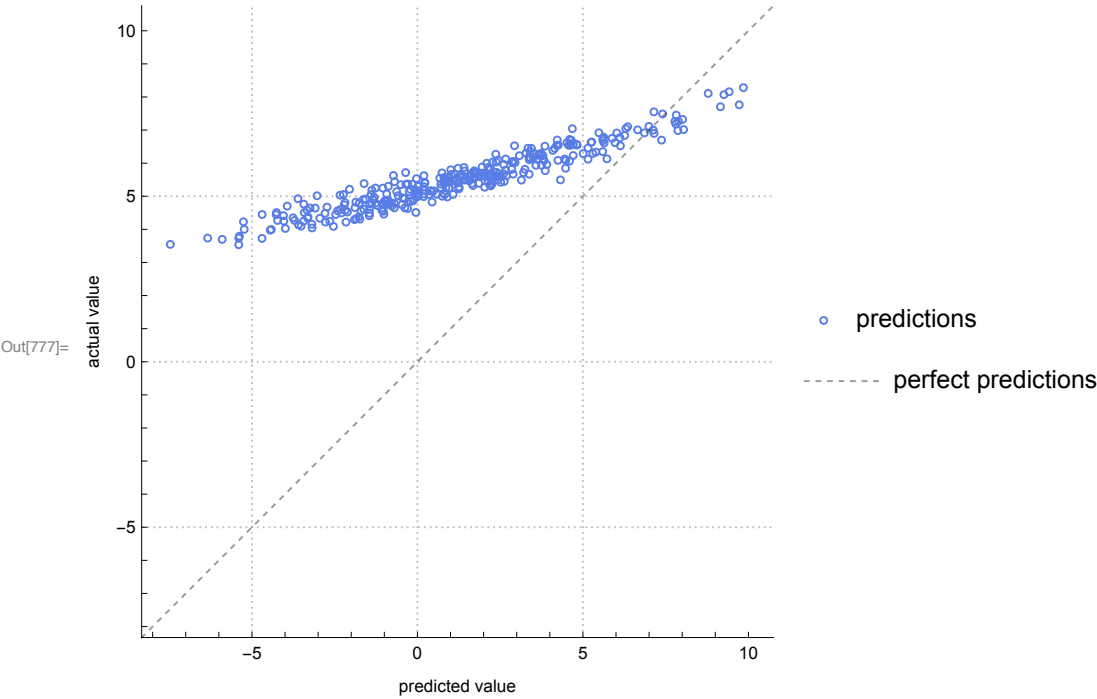
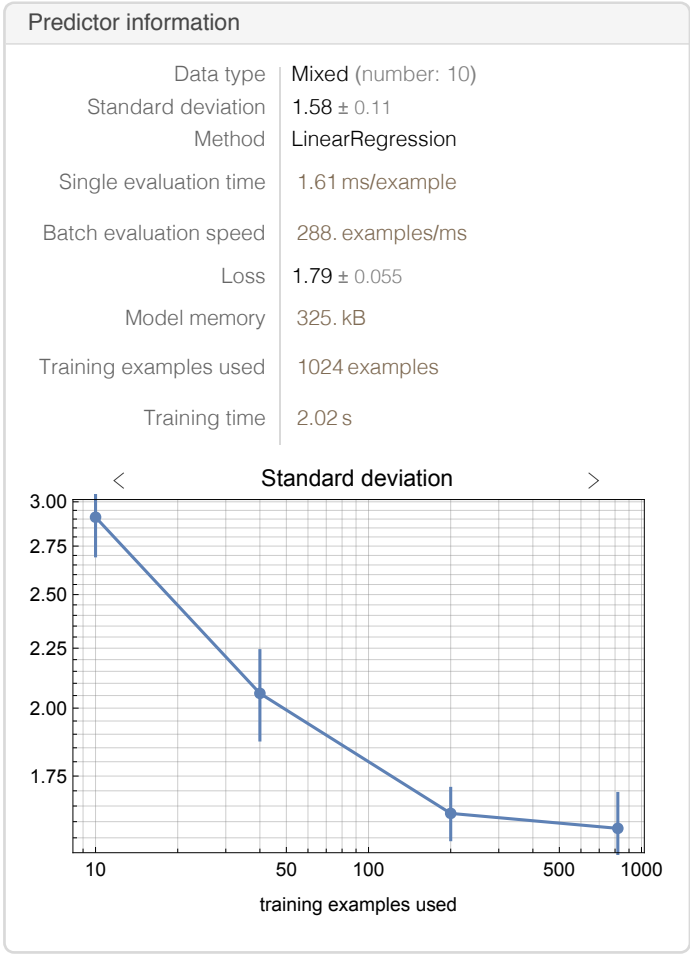


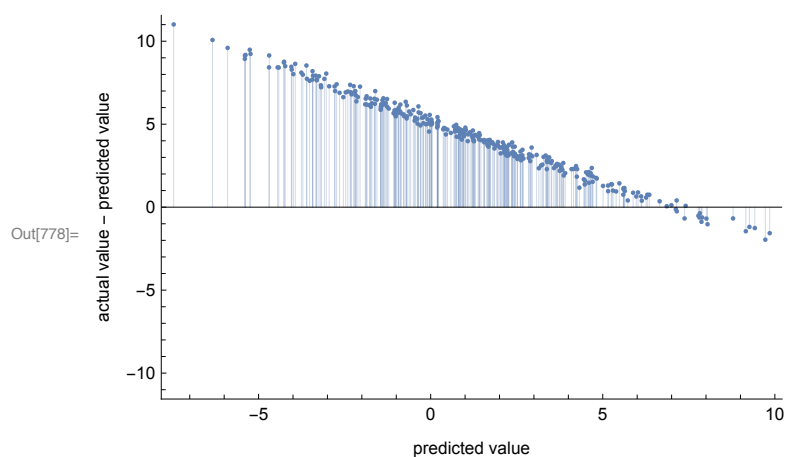


```
In[774]:= pLRv1600 = Predict[finalTrain1600, Method → "LinearRegression"]
pmLRv1600 = PredictorMeasurements[pLRv1600, finaltest1600]
PredictorInformation[pLRv1600]
pmLRv1600["ComparisonPlot"]
pmLRv1600["ResidualPlot"]
```


Out[774]= PredictorFunction [ Input type: Mixed (number: 10)
Method: LinearRegression]

Out[775]= PredictorMeasurementsObject [ Predictor: LinearRegression
Number of test examples: 320]




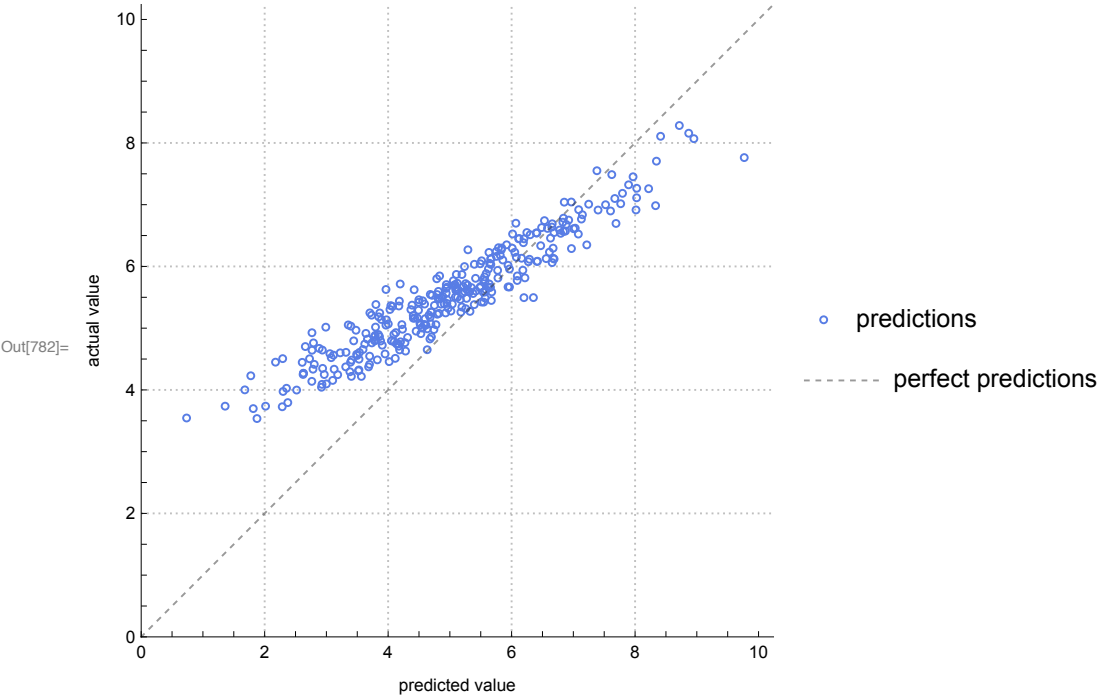
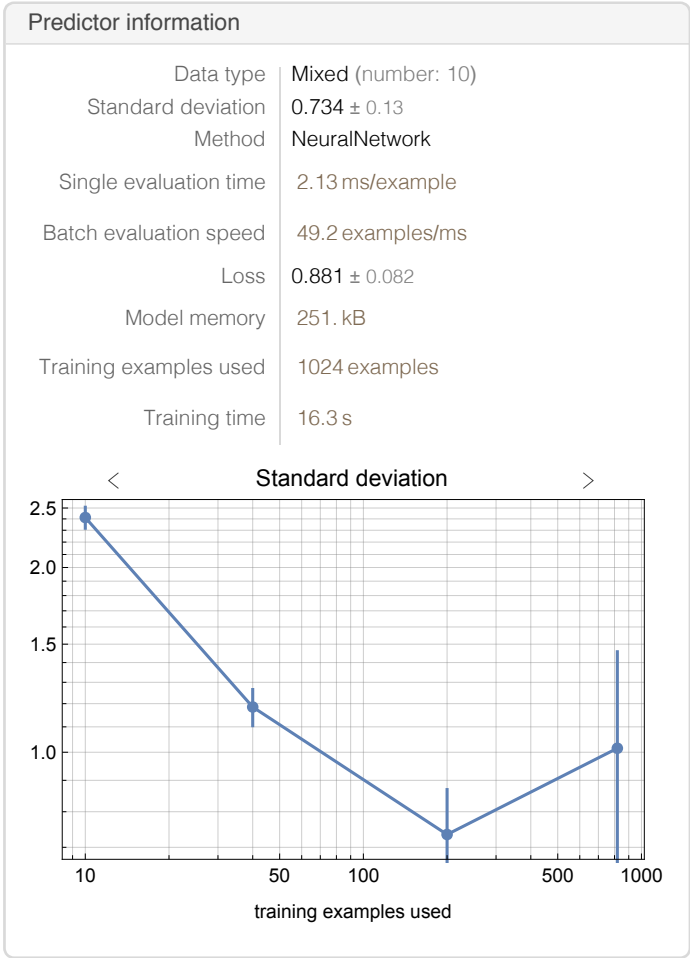


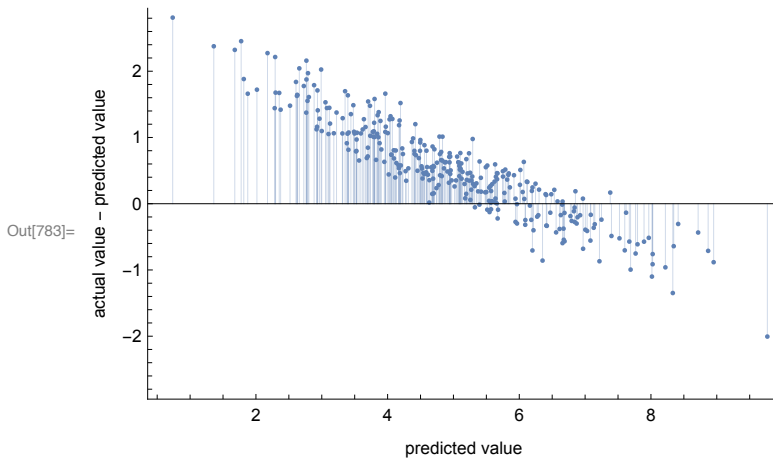
```
In[779]:= pNNv1600 = Predict[finalTrain1600, Method →
  {"NeuralNetwork", "NetworkDepth" → 3, "NetworkType" → "FullyConnected",
    "L2Regularization" → 0.05, MaxTrainingRounds → 1000}]
```

Out[779]= PredictorFunction [ Input type: Mixed (number: 10)
Method: NeuralNetwork]


```
In[780]:= pmNNv1600 = PredictorMeasurements[pNNv1600, finaltest1600]
PredictorInformation[pNNv1600]
pmNNv1600["ComparisonPlot"]
pmNNv1600["ResidualPlot"]
```

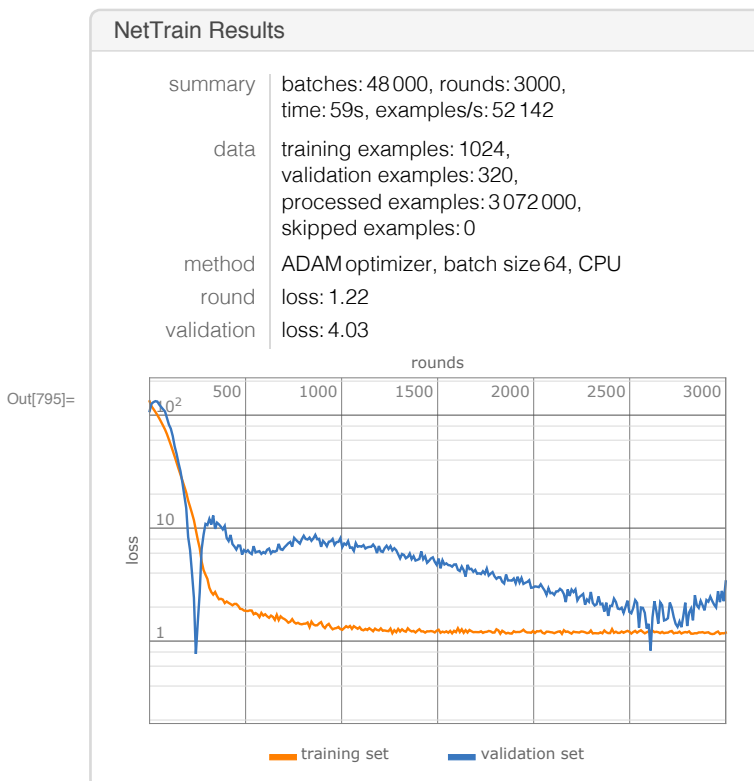
Out[780]= PredictorMeasurementsObject [ Predictor: NeuralNetwork
Number of test examples: 320]





In[794]:= **netSimple1 =**
NetChain[{BatchNormalizationLayer[], Tanh, 100, 100, 100, 100, 100, 100, 100, 100,
BatchNormalizationLayer[], Tanh, 1}, "Input" → 10, "Output" → "Scalar"]
trainedNetSimple1 = NetTrain[netSimple1, finalTrain1600, All,
ValidationSet → finaltest1600, TargetDevice → "CPU", MaxTrainingRounds → 3000,
Method → {"ADAM", "LearningRate" → 0.0001, "L2Regularization" → 0.03}]

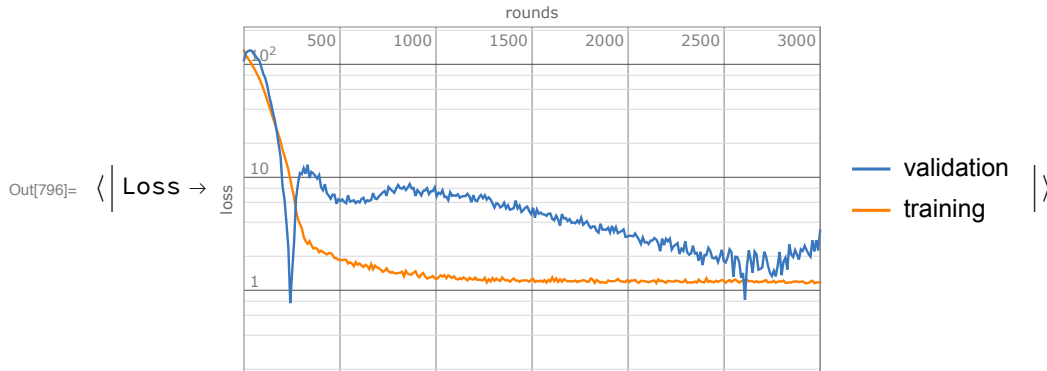
Out[794]= NetChain[
 Input port: vector (size: 10)
Output port: scalar
Number of layers: 12



```

In[796]:= trainedNetSimple1["FinalPlots"]
trainedNetSimple1["RoundMeasurements"]
best = trainedNetSimple1["BestValidationRound"]
trainedNetSimple1["ValidationLossList"][[best]]
NetInformation[trainedNetSimple1["TrainedNet"], "MXNetNodeGraphPlot"]
NetInformation[trainedNetSimple1["TrainedNet"], "SummaryGraphic"]

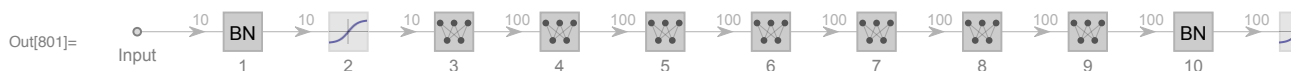
```



Out[797]= $\langle \text{Loss} \rightarrow 1.22379 \rangle$

Out[798]= 2606

Out[799]= 0.304149



```
In[810]:= netSimple2 = NetChain[{BatchNormalizationLayer[], Tanh, 100, 100, 100,  
    100, 100, 100, 100, 100, 100, BatchNormalizationLayer[], Tanh, 1}]  
trainedNetSimple2 = NetTrain[netSimple2, finalTrain1600, All,  
    ValidationSet -> finaltest1600, TargetDevice -> "CPU", MaxTrainingRounds -> 6000,  
    Method -> {"ADAM", "LearningRate" -> 0.0001, "L2Regularization" -> 0.05}]
```

Out[810]= NetChain[

uninitialized

Input port:

Output port:

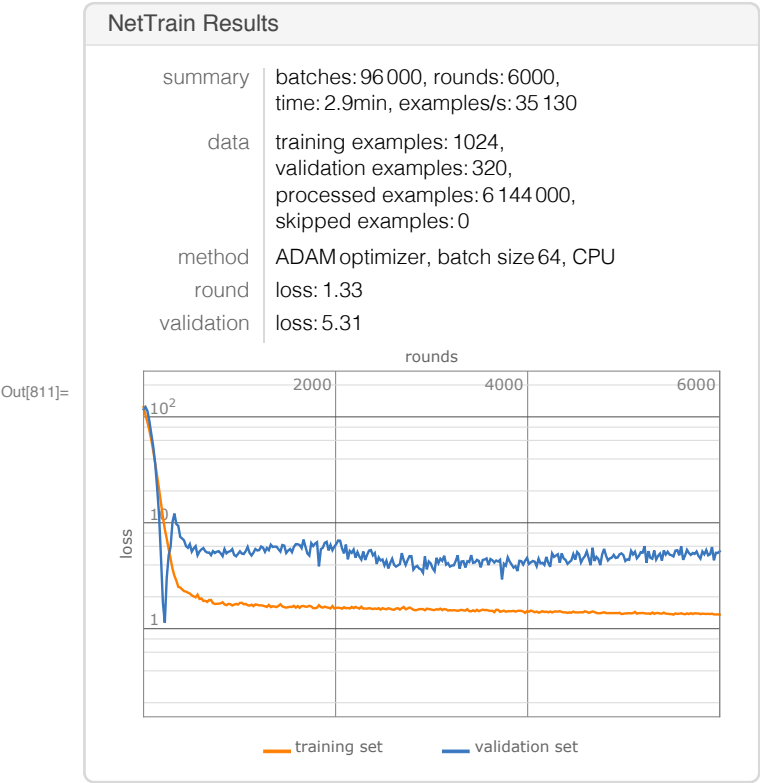
Number of layers:

array of rank ≥ 1

vector (size: 1)

14

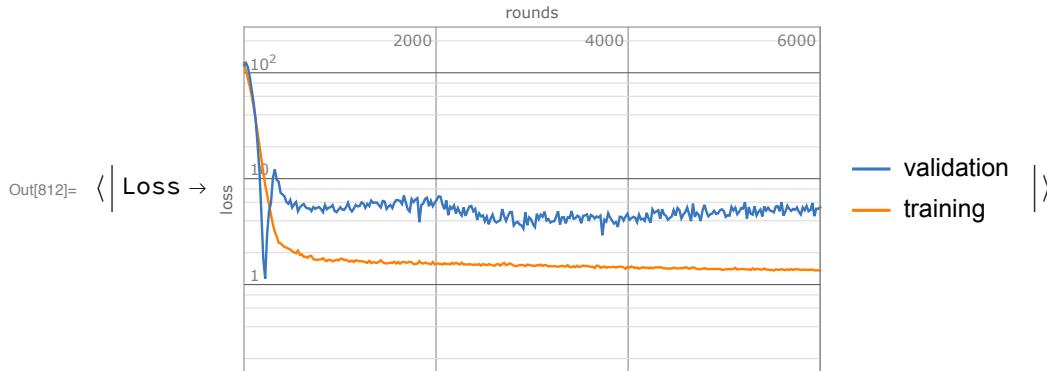
]




```

In[812]:= trainedNetSimple2["FinalPlots"]
trainedNetSimple2["RoundMeasurements"]
best = trainedNetSimple2["BestValidationRound"]
trainedNetSimple2["ValidationLossList"][[best]]
NetInformation[trainedNetSimple2["TrainedNet"], "MXNetNodeGraphPlot"]
NetInformation[trainedNetSimple2["TrainedNet"], "SummaryGraphic"]

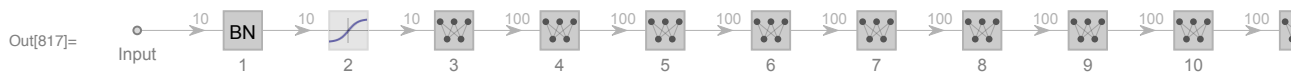
```



Out[813]= $\langle \text{Loss} \rightarrow 1.32644 \rangle$

Out[814]= 3167

Out[815]= 0.234034



```
In[818]:= netSimple3 = NetChain[{BatchNormalizationLayer[], Tanh, 50, 50,  
    50, 50, 50, 50, 50, 50, 50, 50, BatchNormalizationLayer[], Tanh, 1}]  
trainedNetSimple3 = NetTrain[netSimple3, finalTrain1600, All,  
    ValidationSet -> finaltest1600, TargetDevice -> "CPU", MaxTrainingRounds -> 6000,  
    Method -> {"ADAM", "LearningRate" -> 0.0001, "L2Regularization" -> 0.05}]
```

Out[818]= NetChain[

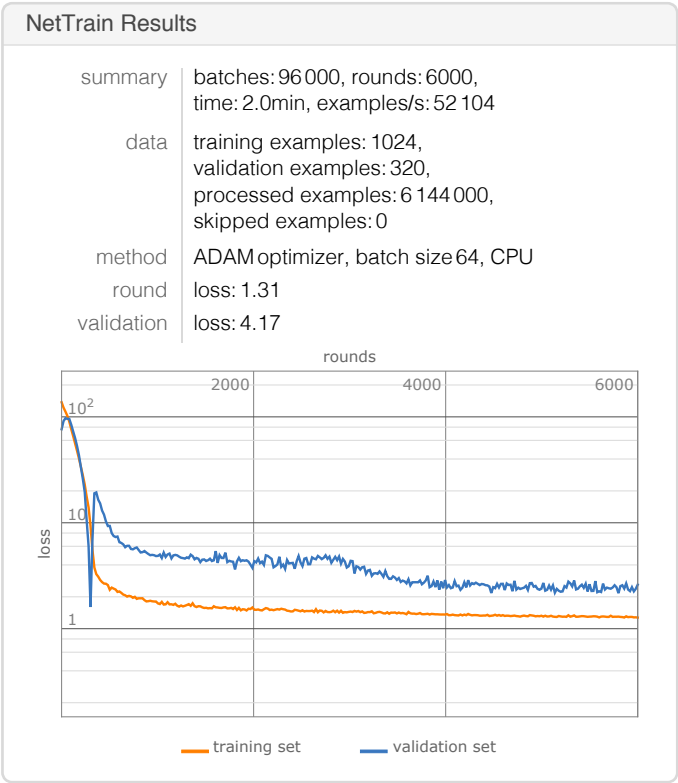
+

uninitialized

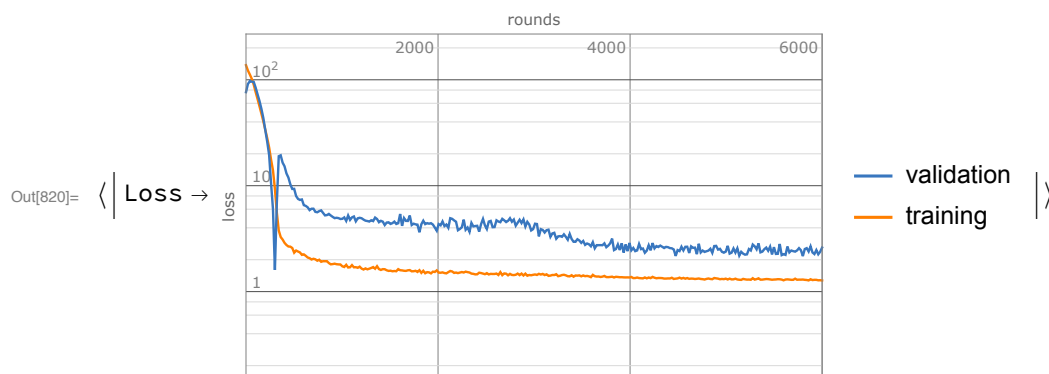
Input port:
Output port:
Number of layers:

array of rank ≥ 1
vector (size: 1)
15

]



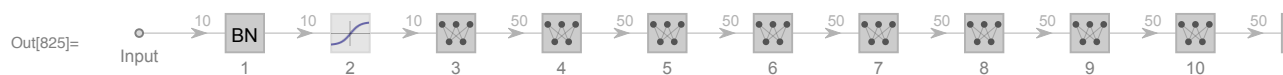
```
In[820]:= trainedNetSimple3["FinalPlots"]
trainedNetSimple3["RoundMeasurements"]
best = trainedNetSimple3["BestValidationRound"]
trainedNetSimple3["ValidationLossList"][[best]]
NetInformation[trainedNetSimple3["TrainedNet"], "MXNetNodeGraphPlot"]
NetInformation[trainedNetSimple3["TrainedNet"], "SummaryGraphic"]
```



Out[821]= $\langle \text{Loss} \rightarrow 1.31077 \rangle$

Out[822]= 4527

Out[823]= 0.223906



```
In[826]:= netSimple4 = NetChain[{BatchNormalizationLayer[], Tanh, 50, 50, 50, 50,  
50, 50, 50, 50, 50, 50, 50, 50, BatchNormalizationLayer[], Tanh, 1}]  
trainedNetSimple4 = NetTrain[netSimple4, finalTrain1600, All,  
ValidationSet -> finaltest1600, TargetDevice -> "CPU", MaxTrainingRounds -> 6000,  
Method -> {"ADAM", "LearningRate" -> 0.0001, "L2Regularization" -> 0.05}]
```

Out[826]= NetChain[

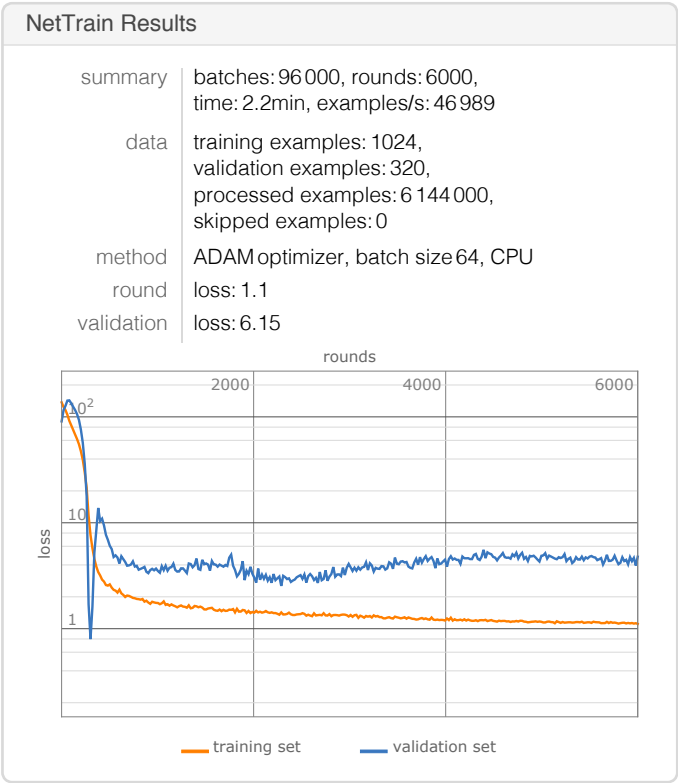
+

uninitialized

Input port:
Output port:
Number of layers:

array of rank ≥ 1
vector (size: 1)
17

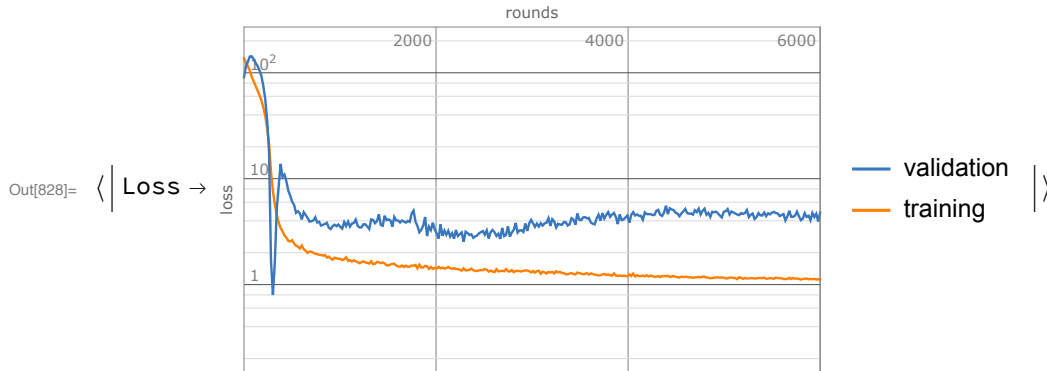
]



```

In[828]:= trainedNetSimple4["FinalPlots"]
trainedNetSimple4["RoundMeasurements"]
best = trainedNetSimple4["BestValidationRound"]
trainedNetSimple4["ValidationLossList"][[best]]
NetInformation[trainedNetSimple4["TrainedNet"], "MXNetNodeGraphPlot"]
NetInformation[trainedNetSimple4["TrainedNet"], "SummaryGraphic"]

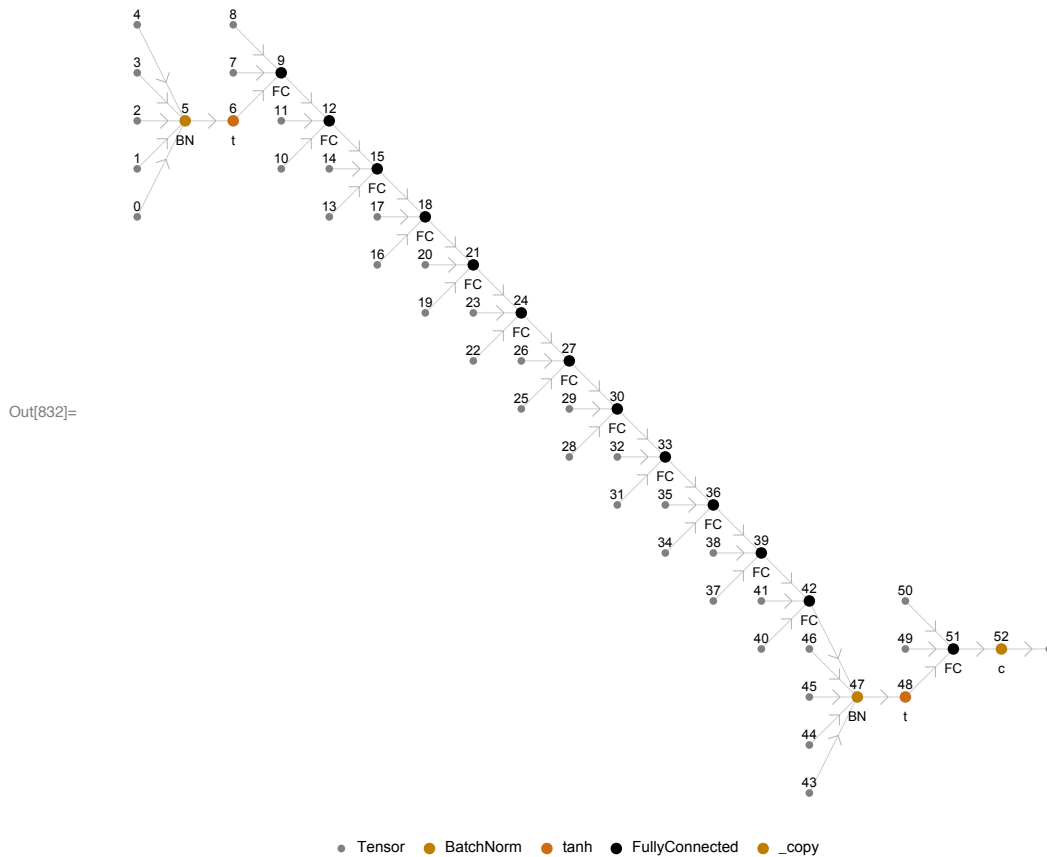
```



Out[829]= $\langle \text{Loss} \rightarrow 1.09542 \rangle$

Out[830]= 4094

Out[831]= 0.228744



```

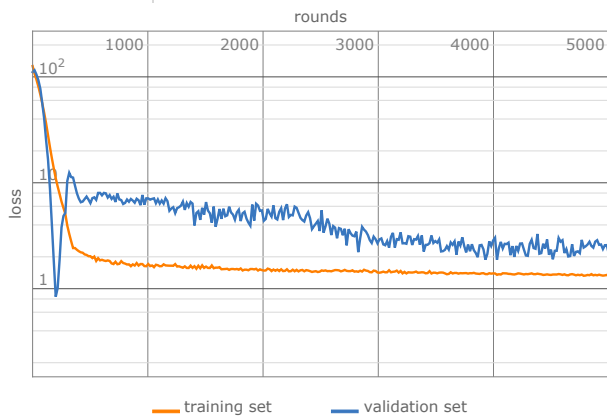
In[834]:= netSimple5 = NetChain[{BatchNormalizationLayer[], Tanh, 100, 100, 100, 100,
    100, 100, 100, 100, 100, 100, BatchNormalizationLayer[], Tanh, 1}]
trainedNetSimple5 = NetTrain[netSimple5, finalTrain1600, All,
    ValidationSet -> finaltest1600, TargetDevice -> "CPU", MaxTrainingRounds -> 5000,
    Method -> {"ADAM", "LearningRate" -> 0.0001, "L2Regularization" -> 0.05}]

```

Out[834]= NetChain[ uninitialized   Input port: array of rank ≥ 1
Output port: vector (size: 1)
Number of layers: 15]

NetTrain Results

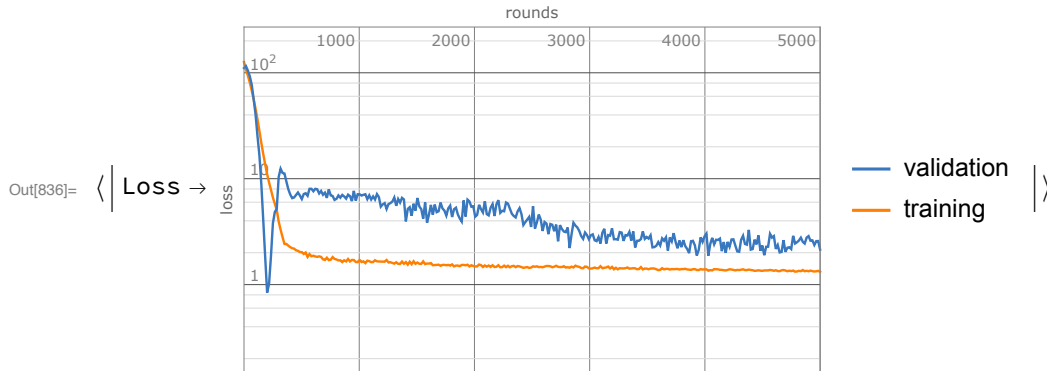
summary	batches: 80 000, rounds: 5000, time: 2.5min, examples/s: 33 834
data	training examples: 1024, validation examples: 320, processed examples: 5 120 000, skipped examples: 0
method	ADAM optimizer, batch size 64, CPU
round	loss: 1.31
validation	loss: 2.42



```

In[836]:= trainedNetSimple5["FinalPlots"]
trainedNetSimple5["RoundMeasurements"]
best = trainedNetSimple5["BestValidationRound"]
trainedNetSimple5["ValidationLossList"][[best]]
NetInformation[trainedNetSimple5["TrainedNet"], "MXNetNodeGraphPlot"]
NetInformation[trainedNetSimple5["TrainedNet"], "SummaryGraphic"]

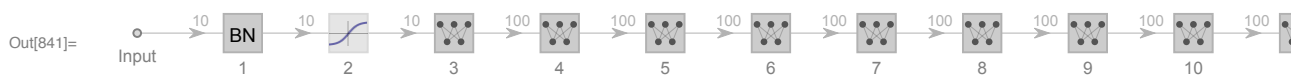
```



Out[837]= $\langle \text{Loss} \rightarrow 1.30938 \rangle$

Out[838]= 3872

Out[839]= 0.214454



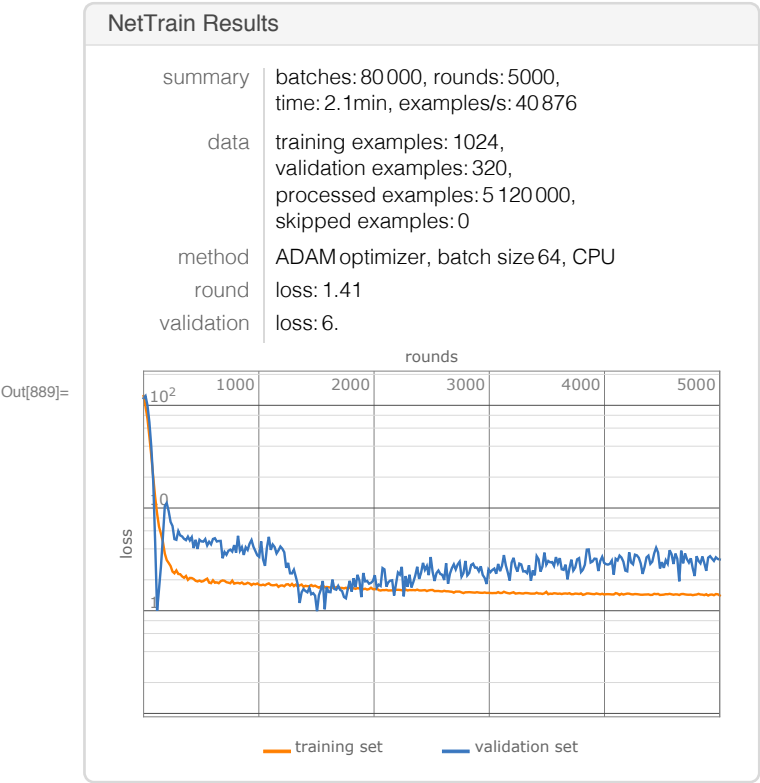
```
In[888]:= netSimple6 = NetChain[{BatchNormalizationLayer[], Tanh, 100, 100,  
    100, 100, 100, 100, 100, 100, BatchNormalizationLayer[], Tanh, 1}]  
trainedNetSimple6 = NetTrain[netSimple6, finalTrain1600, All,  
    ValidationSet -> finaltest1600, TargetDevice -> "CPU", MaxTrainingRounds -> 5000,  
    Method -> {"ADAM", "LearningRate" -> 0.0002, "L2Regularization" -> 0.05}]
```

Out[888]= NetChain[

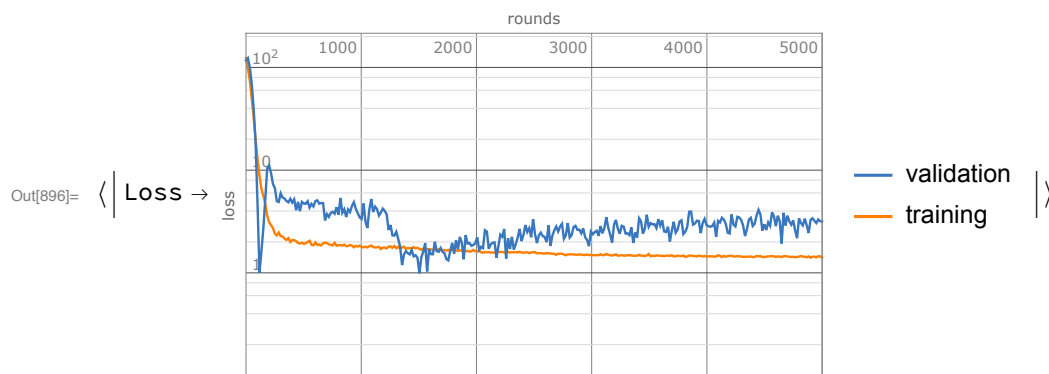
uninitialized

Input port: array of rank ≥ 1
Output port: vector (size: 1)
Number of layers: 13

]




```
In[896]:= trainedNetSimple6["FinalPlots"]
trainedNetSimple6["TotalTrainingTime"]
trainedNetSimple6["RoundMeasurements"]
best = trainedNetSimple6["BestValidationRound"]
trainedNetSimple6["ValidationLossList"][[best]]
NetInformation[trainedNetSimple6["TrainedNet"], "MXNetNodeGraphPlot"]
NetInformation[trainedNetSimple6["TrainedNet"], "SummaryGraphic"]
```

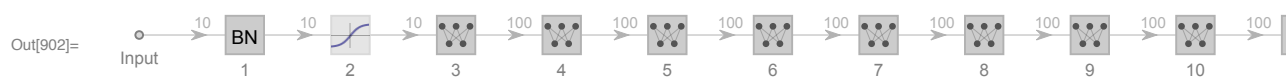


Out[897]= 125.258

```
Out[898]= < | Loss → 1.40556 | >
```

Out[899]= 2098

Out[900]= 0.163367



```

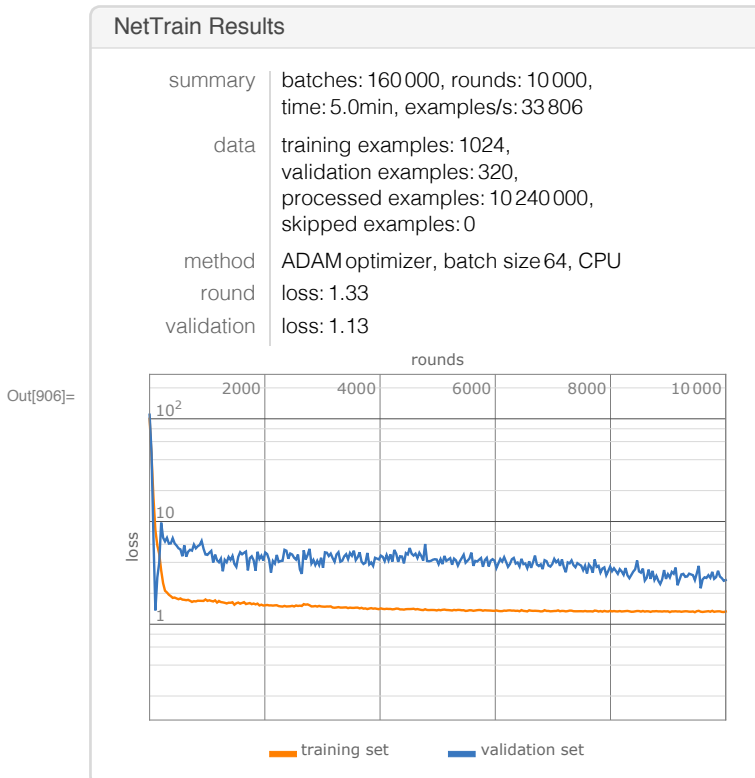
In[905]:= netSimple7 =
  NetChain[{BatchNormalizationLayer[], Tanh, 100, 100, 100, 100, 100, 100, 100, 100,
    100, BatchNormalizationLayer[], Tanh, 1}, "Input" → 10, "Output" → "Scalar"]
trainedNetSimple7 = NetTrain[netSimple7, finalTrain1600, All,
  ValidationSet → finaltest1600, TargetDevice → "CPU", MaxTrainingRounds → 10 000,
  Method → {"ADAM", "LearningRate" → 0.0002, "L2Regularization" → 0.05}]

```

```

Out[905]= NetChain[
  + uninitialized
  Input port: vector (size: 10)
  Output port: scalar
  Number of layers: 14
]

```



```

In[907]:= trainedNetSimple7["FinalPlots"]
trainedNetSimple7["TotalTrainingTime"]
trainedNetSimple7["RoundMeasurements"]
best = trainedNetSimple7["BestValidationRound"]
trainedNetSimple7["ValidationLossList"][[best]]
NetInformation[trainedNetSimple7["TrainedNet"], "MXNetNodeGraphPlot"]
NetInformation[trainedNetSimple7["TrainedNet"], "SummaryGraphic"]

```



302.904

⟨ | Loss → 1.32892 | ⟩

2006


0.186545

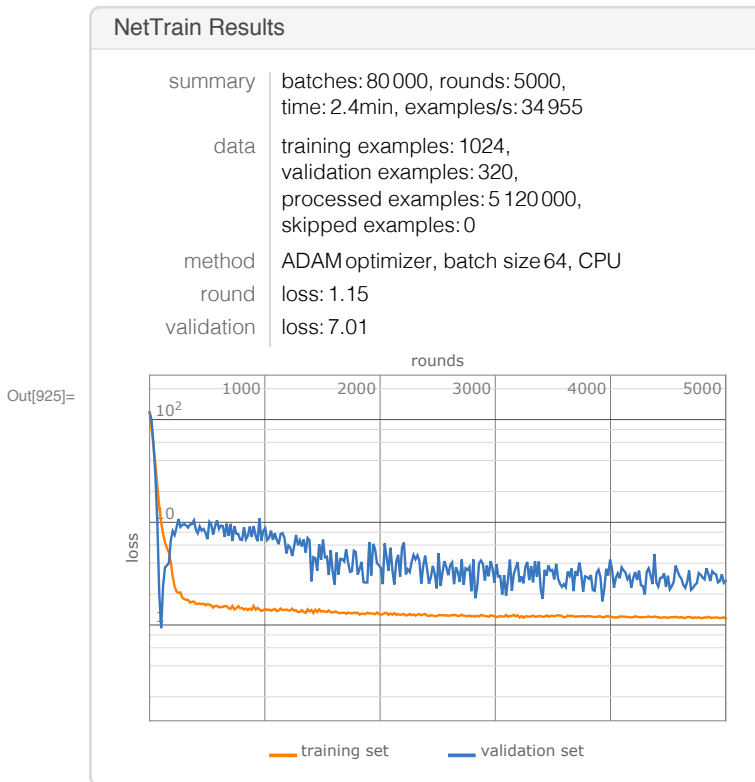


```

In[924]:= net16Simple8 = NetChain[{BatchNormalizationLayer[], Tanh, 100, 100, 100,
  100, 100, 100, 100, 100, 100, 100, BatchNormalizationLayer[], Tanh, 1}]
trainedNet16Simple8 = NetTrain[net16Simple8, finalTrain1600, All,
  ValidationSet → finaltest1600, TargetDevice → "CPU", MaxTrainingRounds → 5000,
  Method → {"ADAM", "LearningRate" → 0.0002, "L2Regularization" → 0.03}]

```

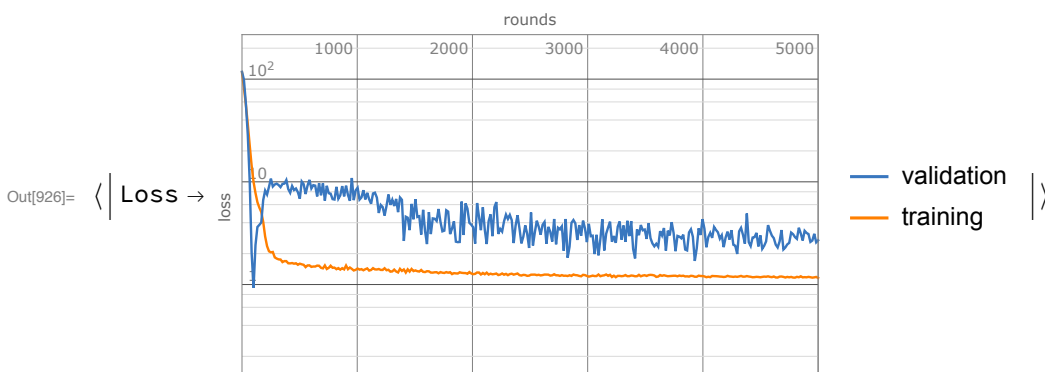
Out[924]= NetChain[
 Input port: array of rank ≥ 1
 Output port: vector (size: 1)
 Number of layers: 15
]



```

In[926]:= trainedNet16Simple8["FinalPlots"]
trainedNet16Simple8["TotalTrainingTime"]
trainedNet16Simple8["RoundMeasurements"]
best = trainedNet16Simple8["BestValidationRound"]
trainedNet16Simple8["ValidationLossList"][[best]]
NetInformation[trainedNet16Simple8["TrainedNet"], "MXNetNodeGraphPlot"]
NetInformation[trainedNet16Simple8["TrainedNet"], "SummaryGraphic"]


```

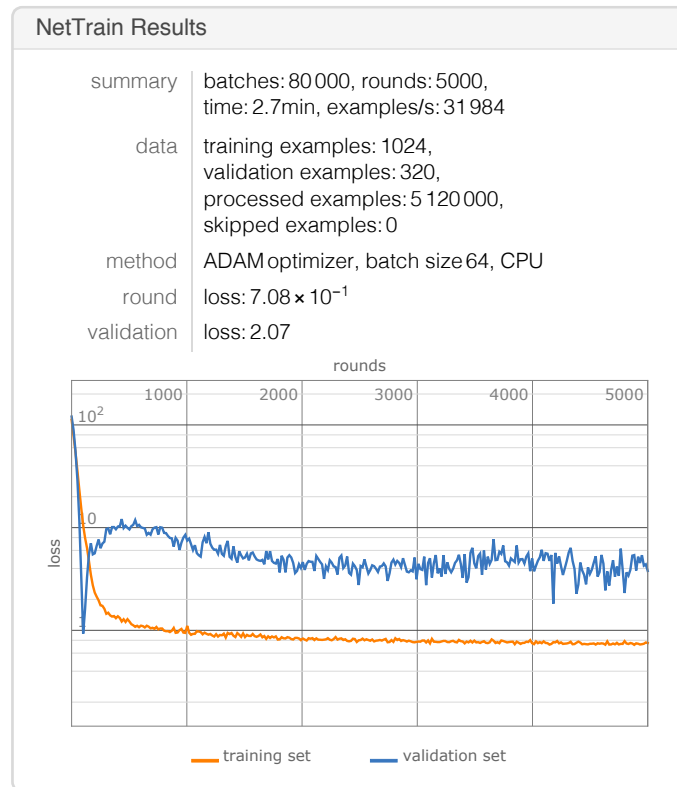



```

In[942]:= net16Simple9 = NetChain[{BatchNormalizationLayer[], Tanh, 100, 100, 100, 100,
    100, 100, 100, 100, 100, 100, 100, BatchNormalizationLayer[], Tanh, 1}]
trainedNet16Simple9 = NetTrain[net16Simple9, finalTrain1600, All,
    ValidationSet → finaltest1600, TargetDevice → "CPU", MaxTrainingRounds → 5000,
    Method → {"ADAM", "LearningRate" → 0.0002, "L2Regularization" → 0.01}]

```

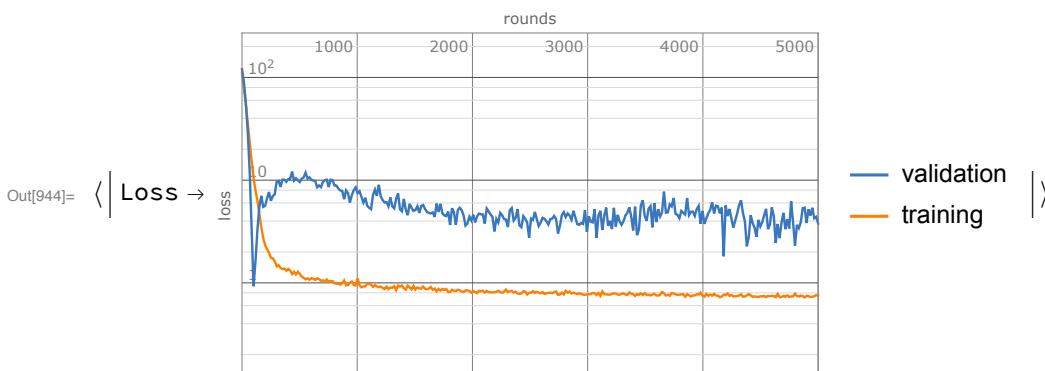
Out[942]= NetChain[
 uninitialized
 Input port: array of rank ≥ 1
 Output port: vector (size: 1)
 Number of layers: 16
]



```

In[944]:= trainedNet16Simple9["FinalPlots"]
trainedNet16Simple9["TotalTrainingTime"]
trainedNet16Simple9["RoundMeasurements"]
best = trainedNet16Simple9["BestValidationRound"]
trainedNet16Simple9["ValidationLossList"][[best]]
NetInformation[trainedNet16Simple9["TrainedNet"], "MXNetNodeGraphPlot"]
NetInformation[trainedNet16Simple9["TrainedNet"], "SummaryGraphic"]

```

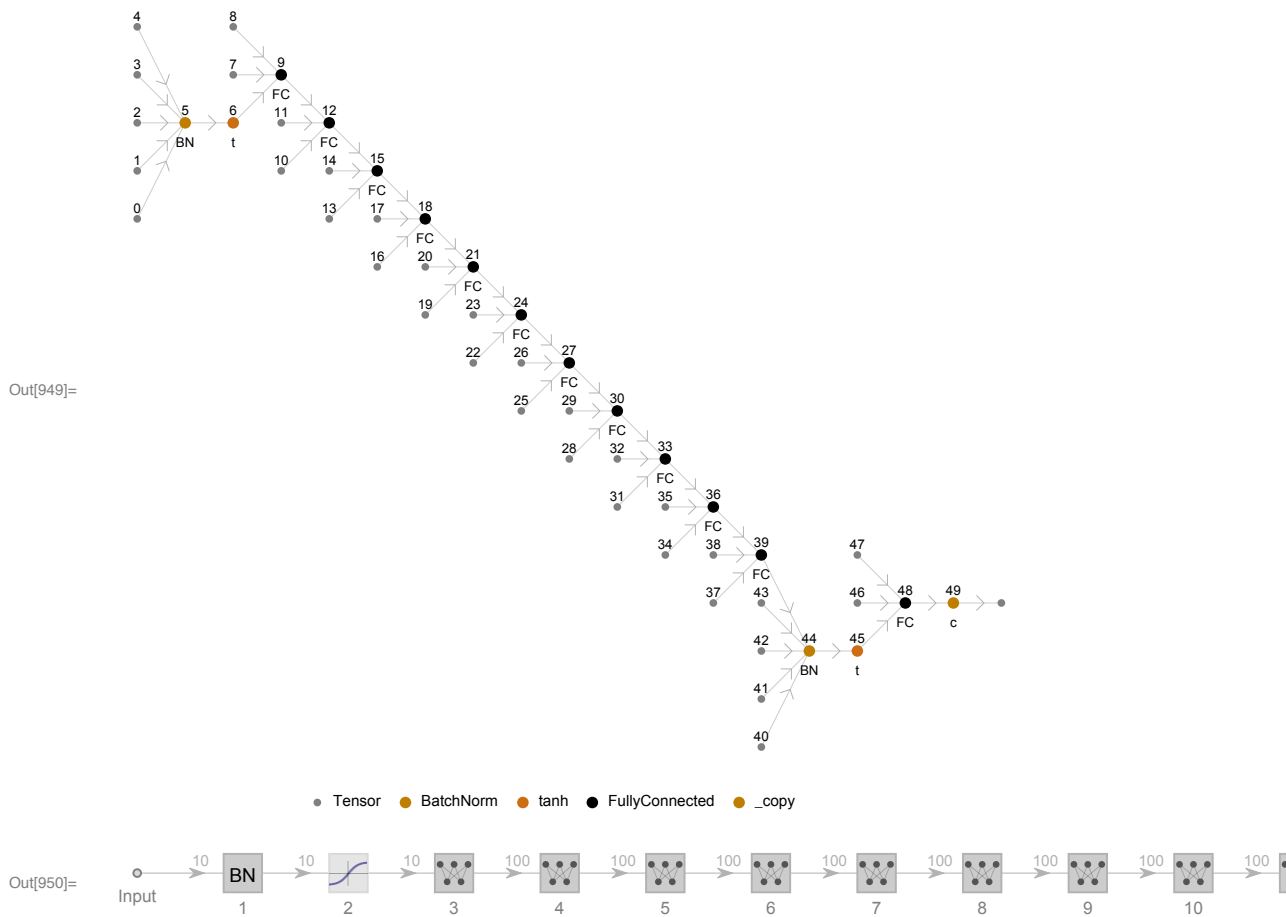


Out[945]= 160.082

Out[946]= $\langle \text{Loss} \rightarrow 0.707874 \rangle$

Out[947]= 4992




Out[948]= 0.171547

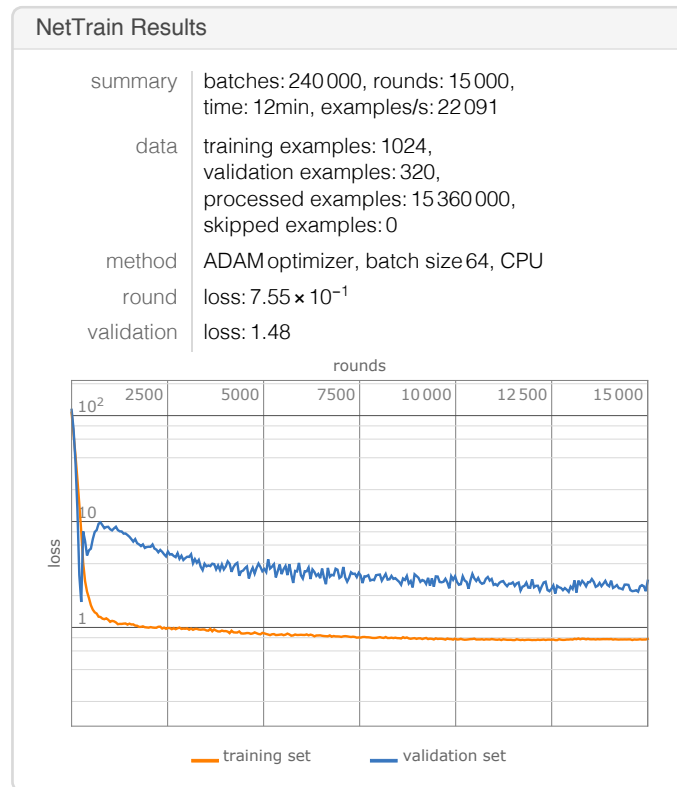


```

In[979]:= net16Simple10 = NetChain[{BatchNormalizationLayer[], Tanh, 100, 100, 100, 100,
    100, 100, 100, 100, 100, 100, 100, BatchNormalizationLayer[], Tanh, 1}]
trainedNet16Simple10 = NetTrain[net16Simple10, finalTrain1600, All,
    ValidationSet → finaltest1600, TargetDevice → "CPU", MaxTrainingRounds → 15 000,
    Method → {"ADAM", "LearningRate" → 0.00008, "L2Regularization" → 0.02}]

```

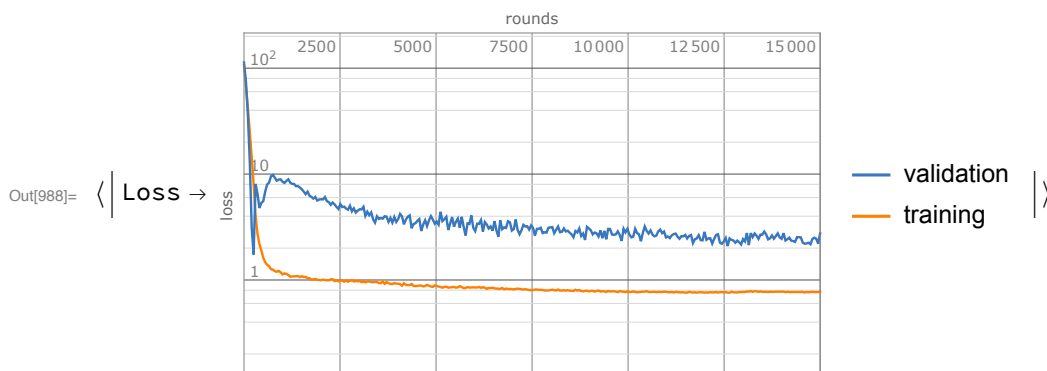
Out[979]= NetChain[ uninitialized   Input port: array of rank ≥ 1
Output port: vector (size: 1)
Number of layers: 16]



```

In[988]:= trainedNet16Simple10["FinalPlots"]
trainedNet16Simple10["TotalTrainingTime"]
trainedNet16Simple10["RoundMeasurements"]
best = trainedNet16Simple10["BestValidationRound"]
trainedNet16Simple10["ValidationLossList"][[best]]
NetInformation[trainedNet16Simple10["TrainedNet"], "MXNetNodeGraphPlot"]
NetInformation[trainedNet16Simple10["TrainedNet"], "SummaryGraphic"]

```

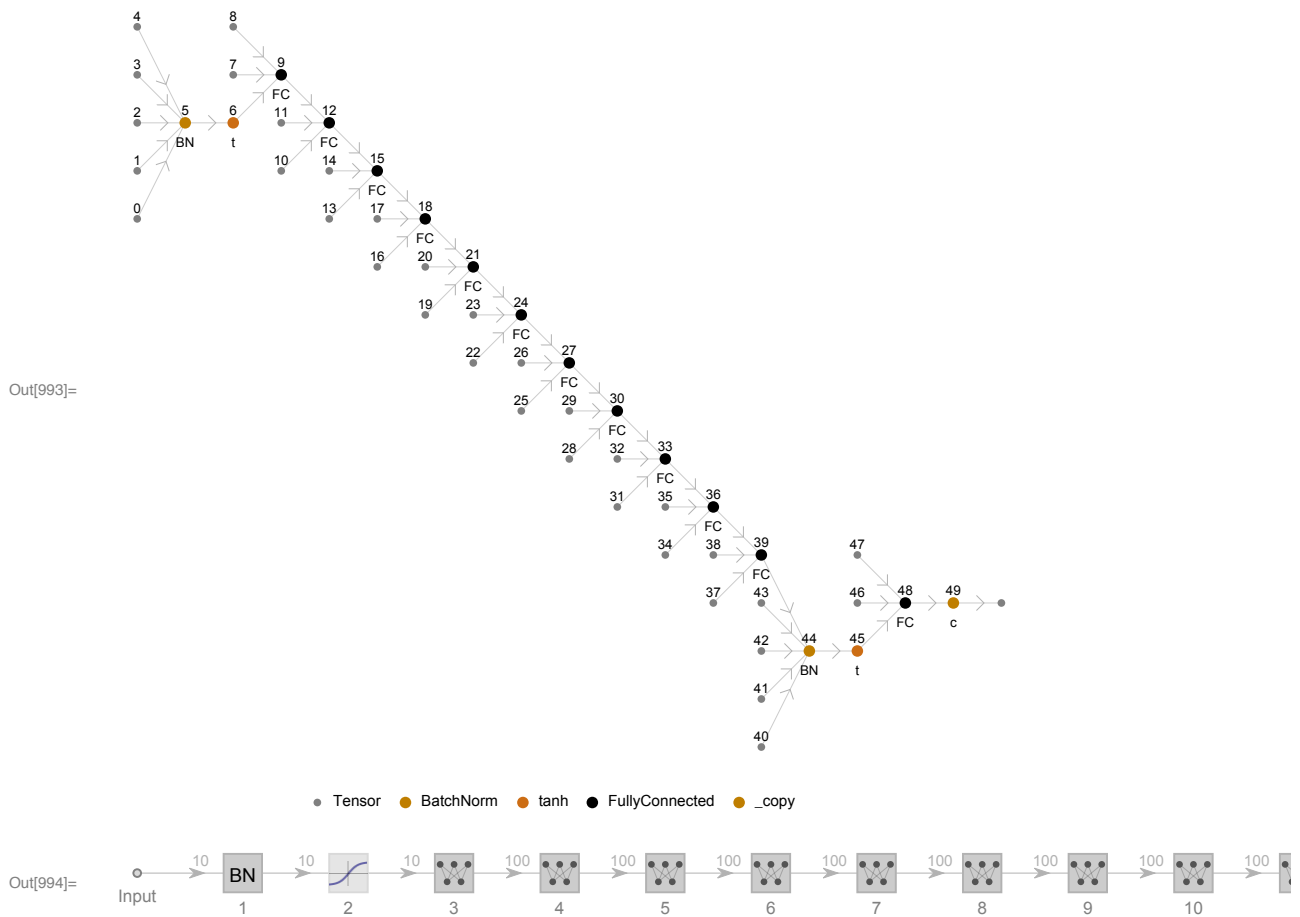


Out[989]= 695.307

Out[990]= $\langle | \text{Loss} \rightarrow 0.755217 | \rangle$

Out[991]= 12 670


Out[992]= 0.188035

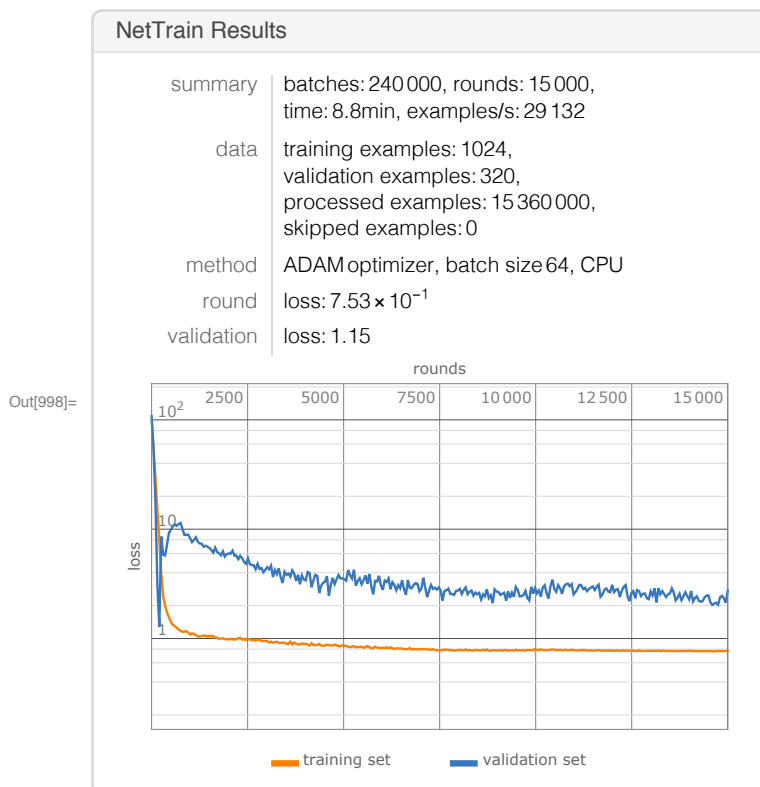


```

In[997]:= net16Simple11 = NetChain[{BatchNormalizationLayer[],
  Tanh, 100, 100, 100, 100, 100, 100, 100, 100, 100, 100, 100,
  BatchNormalizationLayer[], Tanh, 1}, "Input" → 10, "Output" → "Scalar"]
trainedNet16Simple11 = NetTrain[net16Simple11, finalTrain1600, All,
  ValidationSet → finaltest1600, TargetDevice → "CPU", MaxTrainingRounds → 15 000,
  Method → {"ADAM", "LearningRate" → 0.0001, "L2Regularization" → 0.02}]

```

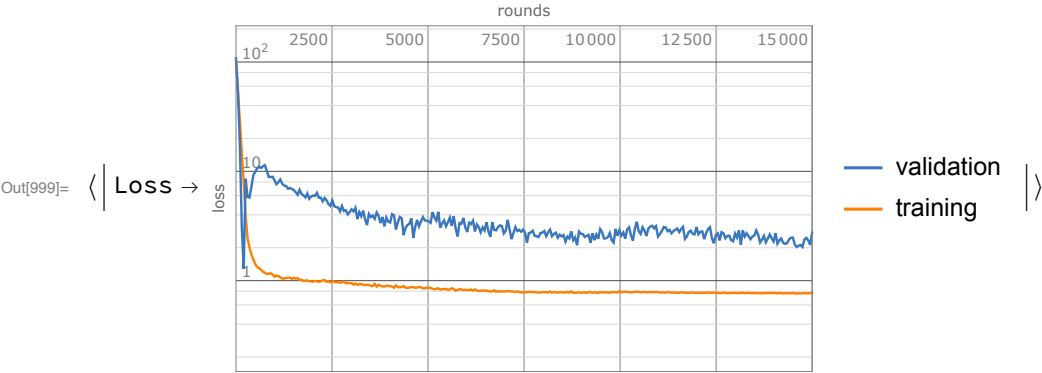
Out[997]= NetChain[
 Input port: vector (size: 10)
 Output port: scalar
 Number of layers: 16
]



```

In[999]:= trainedNet16Simple11["FinalPlots"]
trainedNet16Simple11["TotalTrainingTime"]
trainedNet16Simple11["RoundMeasurements"]
best = trainedNet16Simple11["BestValidationRound"]
trainedNet16Simple11["ValidationLossList"][[best]]
NetInformation[trainedNet16Simple11["TrainedNet"], "MXNetNodeGraphPlot"]
NetInformation[trainedNet16Simple11["TrainedNet"], "SummaryGraphic"]

```

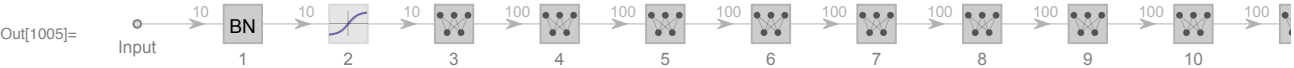
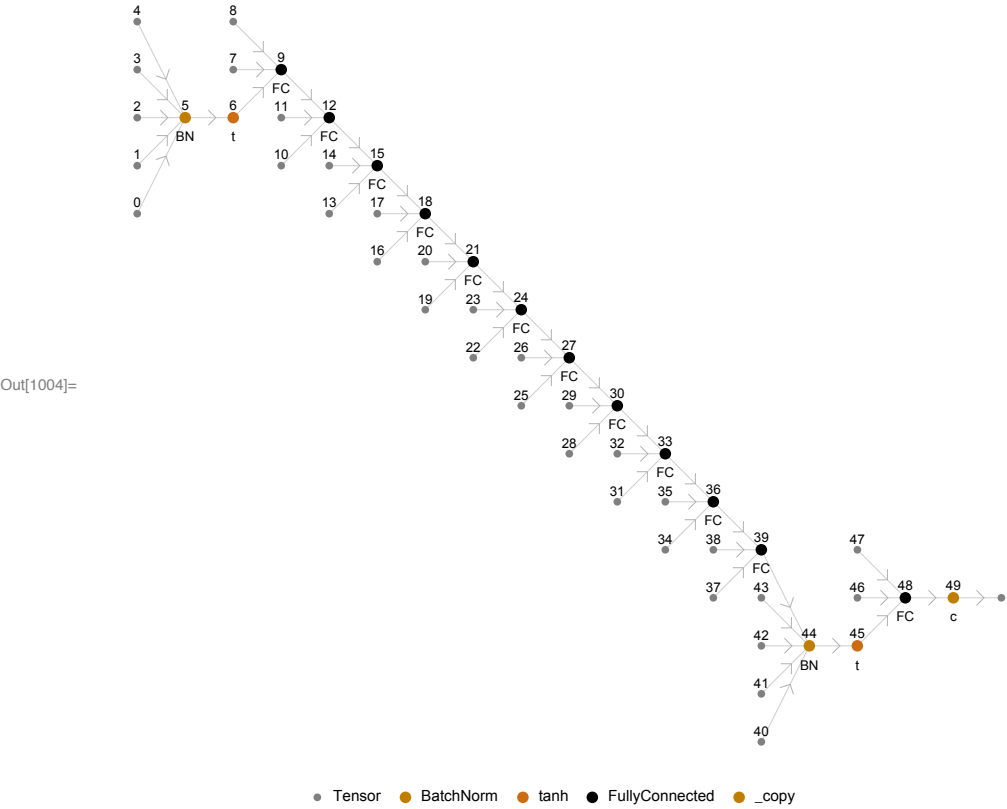


Out[1000]= 527.261

Out[1001]= $\langle | \text{Loss} \rightarrow 0.75316 | \rangle$

Out[1002]= 5110

Out[1003]= 0.209511



MeanSquare

```
In[1112]:= pmNNv1600["MeanSquare"]  
           pmDTv1600["MeanSquare"]  
           pmLRv1600["MeanSquare"]  
           pmRFv1600["MeanSquare"]  
           pmXGTV1600["MeanSquare"]  
           pmGPEv1600["MeanSquare"]  
           pmLRv1600["MeanSquare"]  
           pmNearestv1600["MeanSquare"]
```

```
Out[1112]= 0.806247
```

```
Out[1113]= 2.24735
```

```
Out[1114]= 24.1802
```

```
Out[1115]= 2.65628
```

```
Out[1116]= 2.77351
```

```
Out[1117]= 37.0196
```

```
Out[1118]= 24.1802
```

```
Out[1119]= 7.40404
```