

SVR Flow Diagram. Firstly, the multi-target dataset is divided into m ST datasets,  $\mathcal{D}_1, \mathcal{D}_2, \ldots, \mathcal{D}_m$ . Then m models,  $h_1, h_2, \ldots, h_m$ , are independently trained for each ST dataset.

## Multi-Target Support Vector Regression (SVR)

Input: Training dataset  $\mathcal{D}$ Output: ST models  $h_j, j = 1, \dots, m$ 1: for j = 1 to m do

2:  $\mathcal{D}_j = \{X, Y_j\}$   $\triangleright$  Get ST data

3:  $h_j : X \to \mathbb{R}$   $\triangleright$  Build ST model for the  $j^{th}$  target

4: end for

## **Build Chained Model**

```
Input: Training dataset \mathcal{D}, random chain C
Output: A chained model h_j, j = \{1, \ldots, m\}
 1: \mathcal{D}_1 = \{ X, Y_{C_1} \}
                                                                               ▶ Initialize first dataset
 2: for j=1 to m do
                                                                        \triangleright For each target in chain C
         h_j: \mathcal{D}_j \to \mathbb{R}
 3:
                                                               > Train model on appended dataset
         if j < m then
 4:
               \mathcal{D}_{j+1} = \left\{ \mathcal{D}_j, \mathbf{Y}_{C_j} \right\}
 5:
                                                         > Append new target in chain to dataset
          end if
 7: end for
```

SVRRC Flow Diagram on a dataset with three targets. SVRRC first builds the six random chains of the target's indices (three examples are shown). It then constructs a chained model by proceeding recursively over the chain, building a model, and appending the current target to the input space to predict the next target in the chain.

## Multi-Target SVR with Random-Chains (SVRRC)

**Input:** Training dataset  $\mathcal{D}$ , c random chains  $\mathcal{C}$ 

**Output:** An ensemble of chained models  $h_C$  1: for each  $C \in C$  do

⊳ For each random chain

2:  $h_C \leftarrow \text{buildChainedModel}(\mathcal{D}, C) \triangleright \text{Build a chained model for chain } C$ 

3: end for

$$\mathcal{D}: [\boldsymbol{X}][\boldsymbol{Y}_{1}\boldsymbol{Y}_{2}\boldsymbol{Y}_{3}] \xrightarrow{\text{generate maximum correlation chain}} [1,2,3]$$

$$\frac{\mathbf{E}[(Y_{i}-\mu_{i})(Y_{j}-\mu_{j})]}{\sqrt{\mathbf{E}[(Y_{i}-\mu_{i})(Y_{i}-\mu_{i})]\mathbf{E}[(Y_{j}-\mu_{j})(Y_{j}-\mu_{j})]}}}$$

$$h_{1}: [\boldsymbol{X}] \rightarrow \hat{\boldsymbol{Y}}_{1} \longrightarrow h_{2}: [\boldsymbol{X}\boldsymbol{Y}_{1}] \rightarrow \hat{\boldsymbol{Y}}_{2} \longrightarrow h_{3}: [\boldsymbol{X}\boldsymbol{Y}_{1}\boldsymbol{Y}_{2}] \rightarrow \hat{\boldsymbol{Y}}_{3}$$

SVRCC Flow Diagram on a sample dataset with three targets. SVRCC first finds the direction of maximum correlation among the targets and uses that order as the only chain. It then constructs the chained model, as done in SVRRC.

## Multi-Target SVR with max-Correlation Chain (SVRCC)

1:  $\mathbf{P} = corrcoef(\mathbf{Y})$  ightharpoonupFind correlation coefficient matrix for target variables
2:  $\mathbf{C} = \sum_{i=1}^n \mathbf{P}_{ij}, \forall j=1,\ldots,m$  ightharpoonupSum rows of the correlation matrix
3:  $\mathbf{C} = \mathtt{sort}(\mathbf{C}, \mathbf{decreasing})$  ightharpoonupSort sums in decreasing order
4:  $h_{\mathbf{C}} = \mathtt{buildChainedModel}(\mathcal{D}, \mathbf{C})$  ightharpoonupBuild a max-correlation chained model

Average Relative Root Mean Square Error (aRRMSE) for MT regressors

Datasets	MORF	ST	MTS	MTSC	RC	ERC	ERCC	SVR	SVRRC	SVRCC
Slump	0.6939	0.6886	0.6690	0.6938	0.7019	0.7022	0.6886	0.5765	0.5545	0.5560
Polymer	0.6159	0.5971	0.5778	0.6493	0.6270	0.6544	0.6131	0.5573	0.5253	0.5116
Andro	0.5097	0.5979	0.5155	0.5633	0.5924	0.5885	0.5666	0.4856	0.4651	0.4455
EDM	0.7337	0.7442	0.7413	0.7446	0.7449	0.7452	0.7443	0.7058	0.7070	0.6978
Solar Flare 1	1.3046	1.1357	1.1168	1.0758	0.9951	1.0457	1.0887	0.9917	0.9455	0.9320
Jura	0.5969	0.5874	0.5906	0.5892	0.5910	0.5896	0.5880	0.5952	0.5764	0.5885
Enb	0.1210	0.1165	0.1231	0.1211	0.1268	0.1250	0.1139	0.0977	0.0910	0.0899
Solar Flare 2	1.4167	1.1503	0.9483	1.0840	1.0092	1.0522	1.0928	1.0385	1.0253	1.0298
Wisconsin Cancer	r 0.9413	0.9314	0.9308	0.9336	0.9305	0.9313	0.9323	0.9555	0.9483	0.9427
California Housin	g0.6611	0.6447	0.6974	0.6630	0.7131	0.6690	0.6146	0.6130	0.5945	0.5852
Stock	0.1653	0.1844	0.1787	0.1803	0.1802	0.1789	0.1752	0.1364	0.1337	0.1388
SCPF	0.8273	0.8348	0.8436	0.8308	0.8263	0.8105	0.8290	0.8164	0.8037	0.8013
Puma8NH	0.7858	0.8142	0.8118	0.8311	0.8199	0.8205	0.8207	0.7655	0.7744	0.7676
Friedman	0.9394	0.9214	0.9231	0.9210	0.9231	0.9209	0.9204	0.9218	0.9208	0.9196
Puma32H	0.9406	0.8713	0.8727	0.8791	0.8752	0.8729	0.8740	0.9364	0.9367	0.9319
Water Quality	0.8994	0.9085	0.9109	0.9093	0.9121	0.9097	0.9057	0.9343	0.9310	0.9045
M5SPEC	0.5910	0.5523	0.5974	0.5671	0.5552	0.5542	0.5558	0.2951	0.2935	0.2925
MP5SPEC	0.5522	0.5120	0.5683	0.5133	0.5145	0.5143	0.5119	0.2484	0.2323	0.2358
MP6SPEC	0.5553	0.5152	0.5686	0.5119	0.5198	0.5187	0.5109	0.2850	0.2669	0.2623
ATP7d	0.5563	0.5308	0.5141	0.5142	0.5558	0.5397	0.5182	0.5455	0.5371	0.5342
OES97	0.5490	0.5230	0.5229	0.5217	0.5239	0.5237	0.5222	0.4641	0.4618	0.4635
Osales	0.7596	0.7471	0.7086	0.7268	0.8318	0.7258	0.7101	0.7924	0.7924	0.7811
ATP1d	0.4173	0.3732	0.3733	0.3712	0.3790	0.3696	0.3721	0.3773	0.3707	0.3775
OES10	0.4518	0.4174	0.4176	0.4171	0.4178	0.4180	0.4166	0.3570	0.3555	0.3538
Average	0.6910	0.6625	0.6551	0.6589	0.6611	0.6575	0.6536	0.6039	0.5935	0.5893
Ranks	7.5000	5.7708	5.9375	6.1667	7.4375	6.3750	4.9792	4.7708	3.2708	2.7917

Run Time (seconds) for MT regressors

Datasets	MORF	ST	MTS	MTSC	RC	ERC	ERCC	SVR	SVRRC	SVRCC
Slump	38.1	2.6	9.9	15.9	1.8	11.1	50.5	0.6	1.9	0.7
Polymer	7.6	2.7	9.1	15.5	1.9	14.9	80.5	0.5	2.6	0.5
Andro	25.7	4.4	15.0	34.2	3.4	33.2	197.9	1.1	6.2	1.1
EDM	24.8	2.8	9.4	18.1	2.1	5.8	19.0	0.9	1.0	0.9
Solar Flare 1	34.1	3.5	13.6	26.7	2.7	17.7	86.9	2.3	9.3	2.6
Jura	64.3	7.9	31.8	74.3	6.4	43.5	254.2	4.7	18.7	5.3
Enb	71.4	6.6	26.1	63.6	5.4	15.6	69.6	11.3	17.7	15.9
Solar Flare 2	55.4	7.4	30.7	68.0	6.3	42.9	241.5	9.4	53.5	15.6
Wisconsin Cancer	51.4	6.1	21.9	53.7	4.9	14.8	61.6	2.0	2.4	2.0
California Housing	g 93.0	9.7	34.8	75.9	8.2	21.3	102.0	15.8	25.2	23.6
Stock	93.7	11.7	46.8	96.7	11.0	75.4	427.3	18.5	90.5	26.3
SCPF	66.3	19.3	65.9	176.3	15.0	104.2	734.2	32.8	162.8	48.8
Puma8NH	130.4	29.7	106.7	288.6	27.9	201.6	1227.7	94.1	516.6	177.1
Friedman	79.5	27.0	81.2	258.3	25.0	273.7	2871.6	12.3	322.3	18.8
Puma32H	93.9	68.1	181.0	635.0	87.7	667.9	6087.0	32.2	1018.7	53.1
Water Quality	108.4	93.1	262.1	912.3	127.2	925.4	10993.3	110.2	2567.9	189.5
M5SPEC	89.8	68.9	166.3	604.6	73.7	262.3	3132.1	39.2	546.7	45.1
MP5SPEC	84.5	94.6	221.2	888.3	91.5	557.0	6864.1	49.3	1132.1	58.4
MP6SPEC	90.3	93.4	212.6	871.0	89.1	557.6	6761.3	47.2	1227.1	58.5
ATP7d	70.5	262.6	452.1	2319.8	242.1	1779.2	24373.8	80.0	1897.4	136.5
OES97	83.4	485.3	1146.6	4928.9	499.8	5315.0	58072.1	148.2	3759.1	342.6
Osales	92.0	1094.8	2340.7	8322.2	986.5	11361.2	122265.3	437.0	4830.1	843.6
ATP1d	70.7	272.9	476.5	2568.9	261.9	2138.9	26768.9	95.0	2127.8	174.4
OES10	90.0	738.9	1633.6	6682.9	688.5	7150.8	83533.1	229.1	5419.4	577.1
Average	71.2	142.2	316.5	1250.0	136.2	1316.3	14803.2	61.4	1073.2	117.4
Ranks	5.5	3.71	6.0	8.29	3.0	7.08	9.92	1.88	6.71	2.92