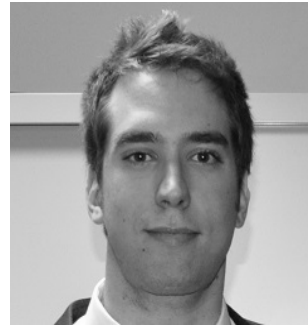


# SGP-DT: Semantic Genetic Programming Based on Dynamic Targets



**Stefano Ruberto**



**Valerio Terragni**



**Jason H. Moore**



# Symbolic Regression

## Training Cases

$$\begin{array}{cccccc} X_1 & X_2 & X_3 & \dots & X_n & \hat{Y}_1 \\ X_1 & X_2 & X_3 & \dots & X_n & \hat{Y}_2 \\ & & & \dots & & \dots \\ X_1 & X_2 & X_3 & \dots & X_n & \hat{Y}_m \end{array}$$

# Symbolic Regression

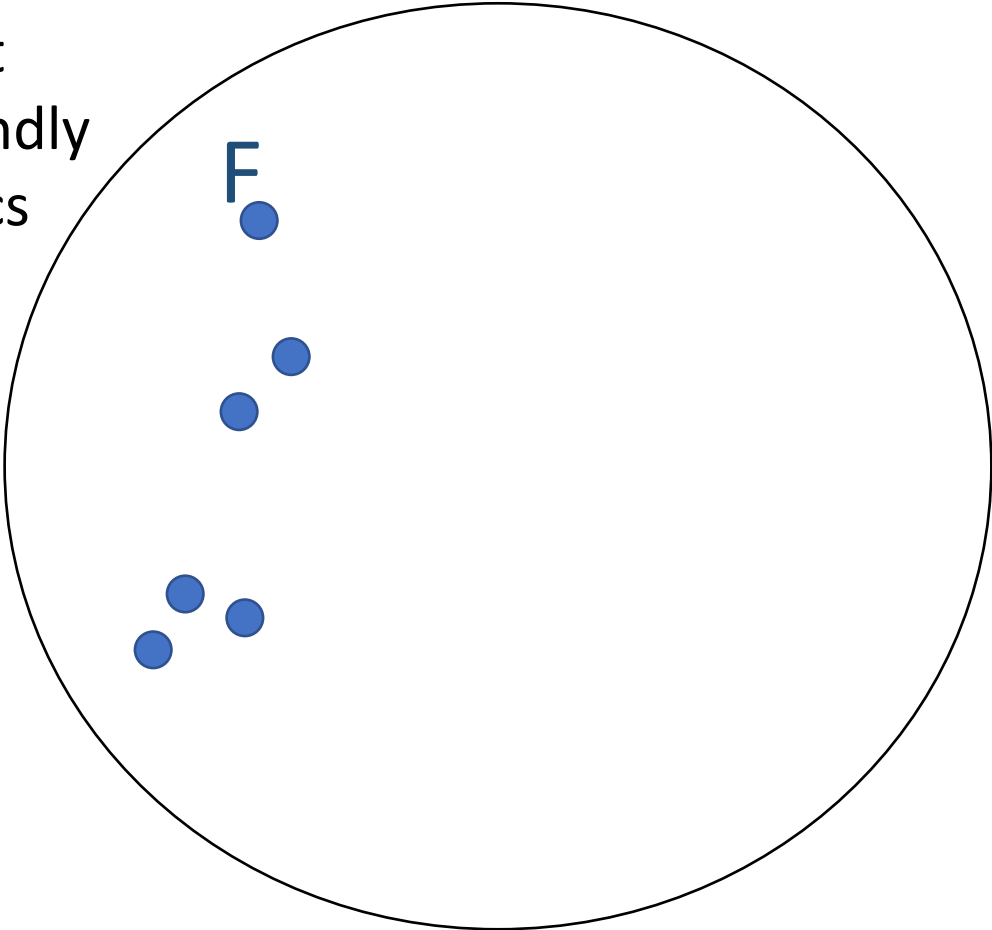
## Training Cases

$$\begin{aligned} F(x_1 x_2 x_3 \dots x_n) &= \hat{y}_1 \\ F(x_1 x_2 x_3 \dots x_n) &= \hat{y}_2 \\ &\dots \\ F(x_1 x_2 x_3 \dots x_n) &= \hat{y}_m \end{aligned}$$

# Genetic Programming (GP)

## (Semantic) Search Space

GP operates at syntactic level blindly to the semantics



## Training Cases

$$F(x_1 x_2 x_3 \dots x_n) = y_1$$

$$F(x_1 x_2 x_3 \dots x_n) = y_2$$

.....

$$F(x_1 x_2 x_3 \dots x_n) = y_m$$

# Semantic Genetic Programming (SGP)


## Training Cases

$$F(x_1 x_2 x_3 \dots x_n) = y_1$$

$$F(x_1 x_2 x_3 \dots x_n) = y_2$$

.....

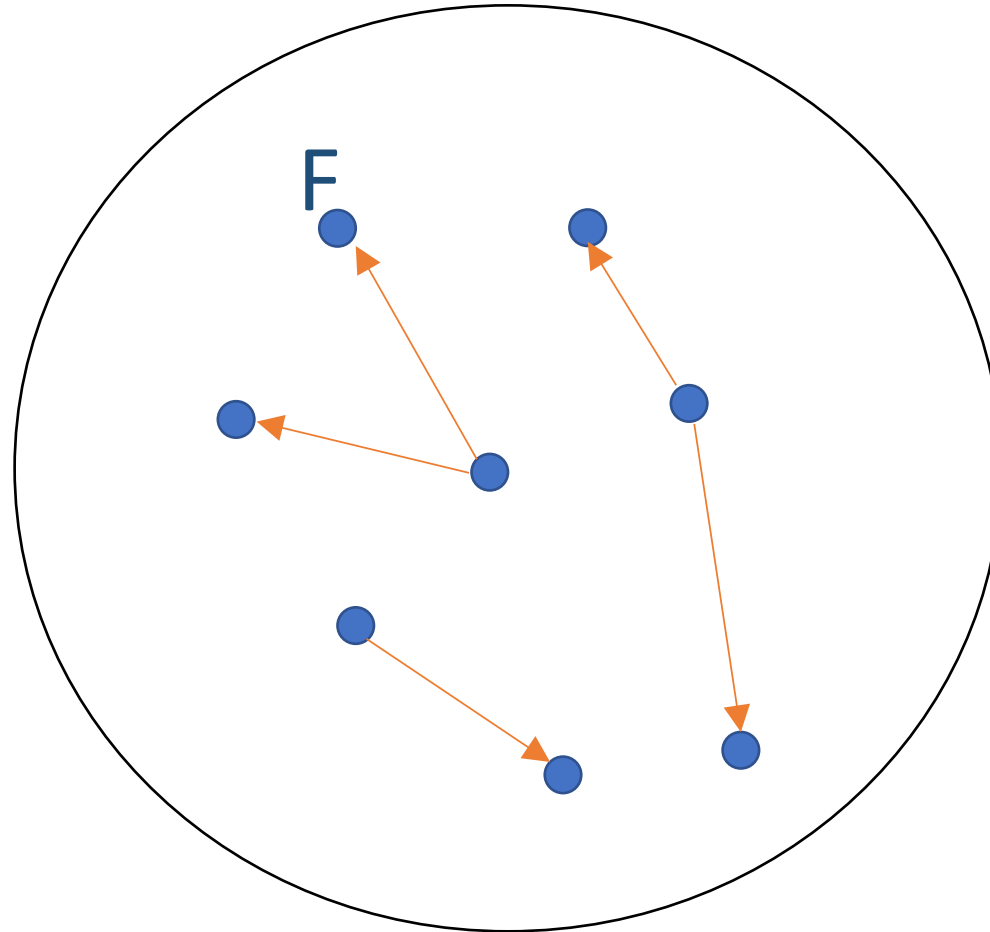
...

$$F(x_1 x_2 x_3 \dots x_n) = y_m$$


$$\text{sem}(F) = (y_1, y_2, \dots y_m)$$

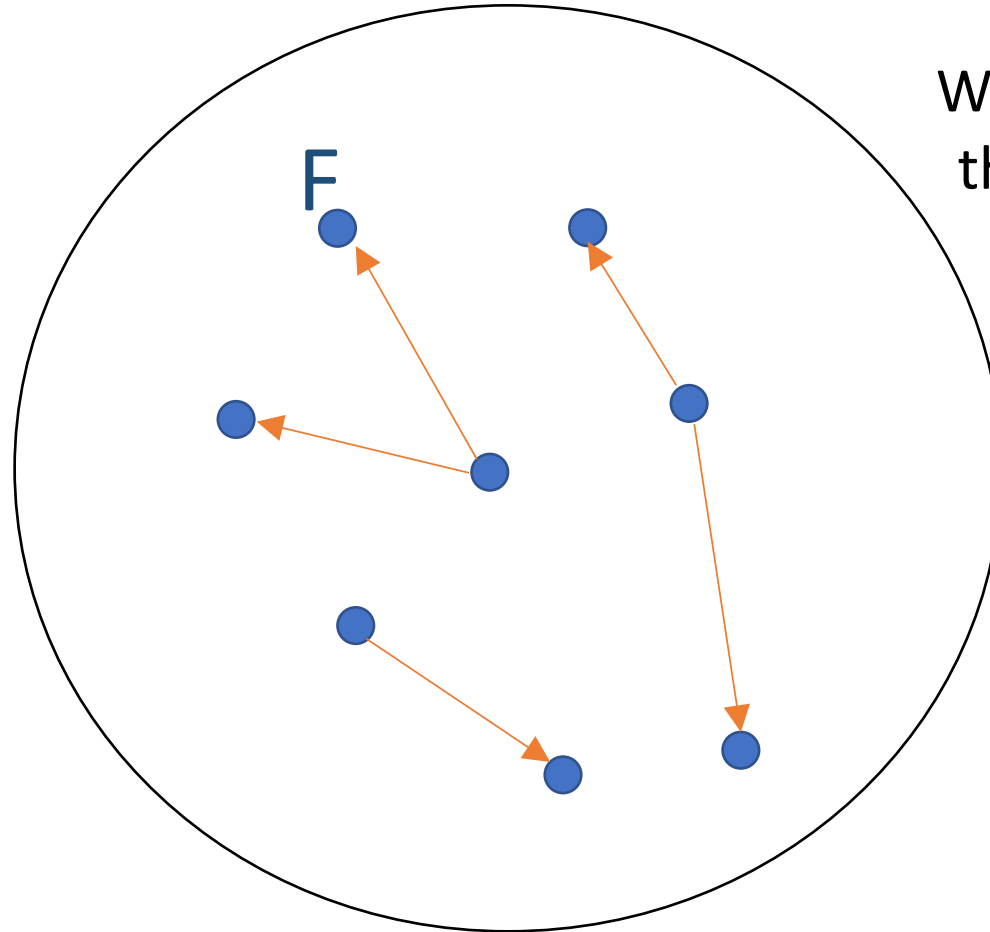
# Semantic Genetic Programming (SGP)

## (Semantic) Search Space



# Semantic Genetic Programming (SGP)

## (Semantic) Search Space



We need SGP approaches that effectively navigate the semantic space



# The Goals of SGP Approaches

- computational efficient
- alleviate the bloat problem
- guarantee semantic properties of the offspring

# The Goals of SGP Approaches

- computational efficient
- alleviate the bloat problem
- guarantee semantic properties of the offspring

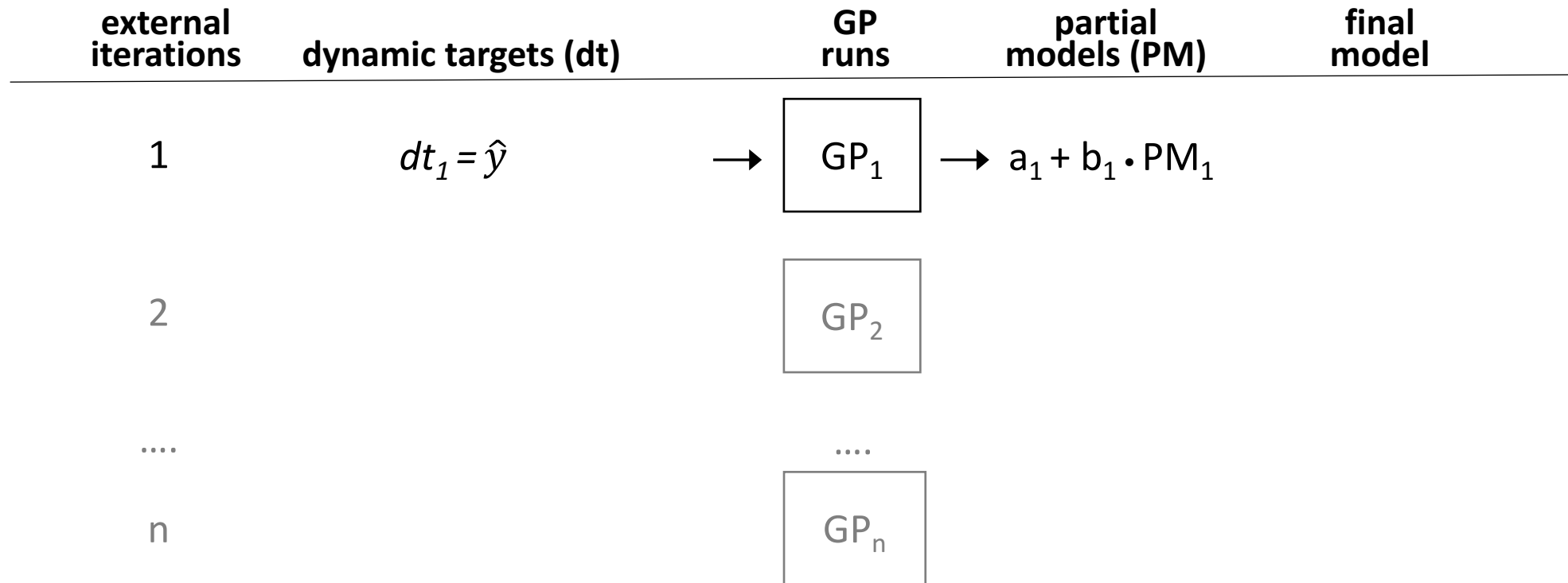
It is difficult to achieve all of these goals at the same time!

# SGP-DT: SGP Based on Dynamic Targets

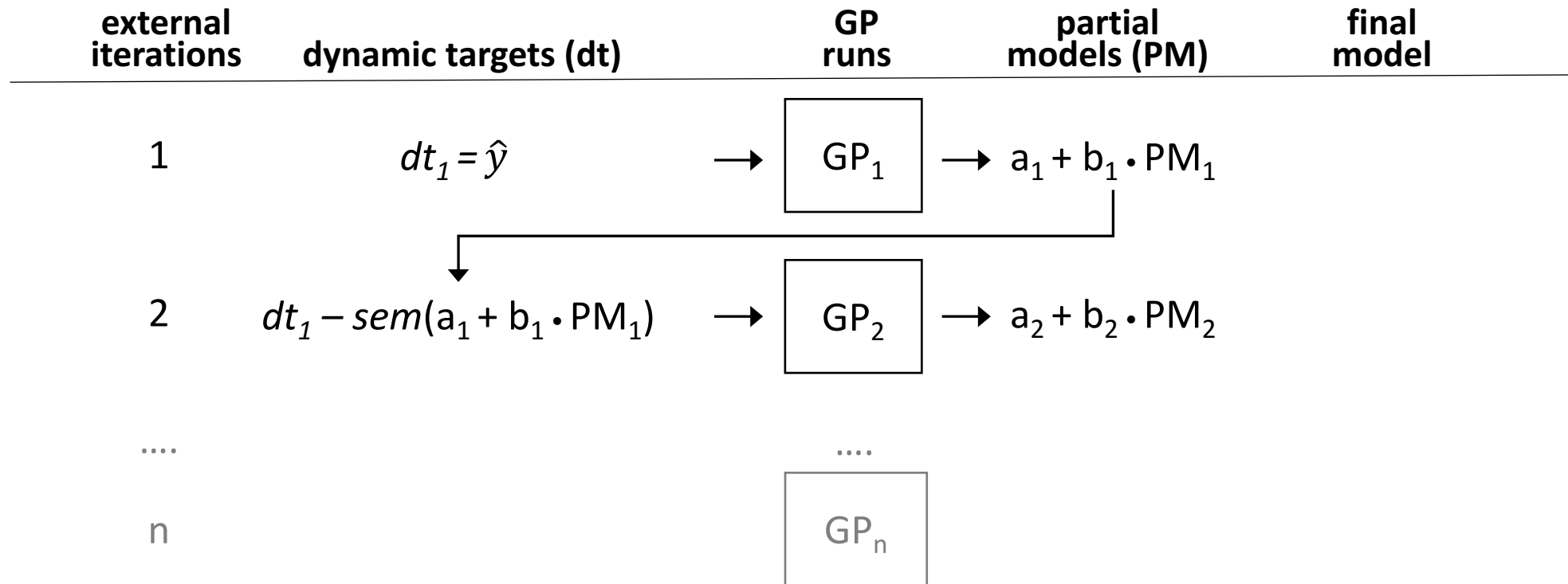
# SGP-DT: SGP Based on Dynamic Targets

external iterations	dynamic targets (dt)	GP runs	partial models (PM)	final model
1		GP <sub>1</sub>		
2		GP <sub>2</sub>		
....		....		
n		GP <sub>n</sub>		

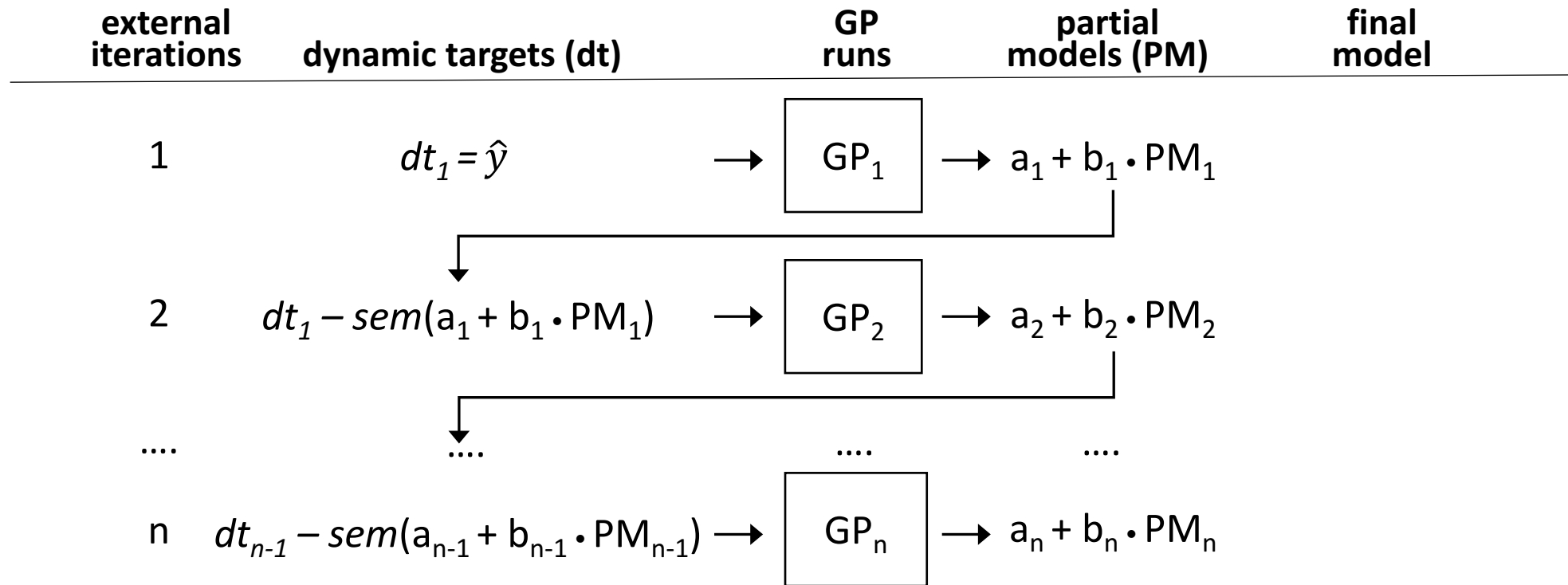
# SGP-DT: SGP Based on Dynamic Targets



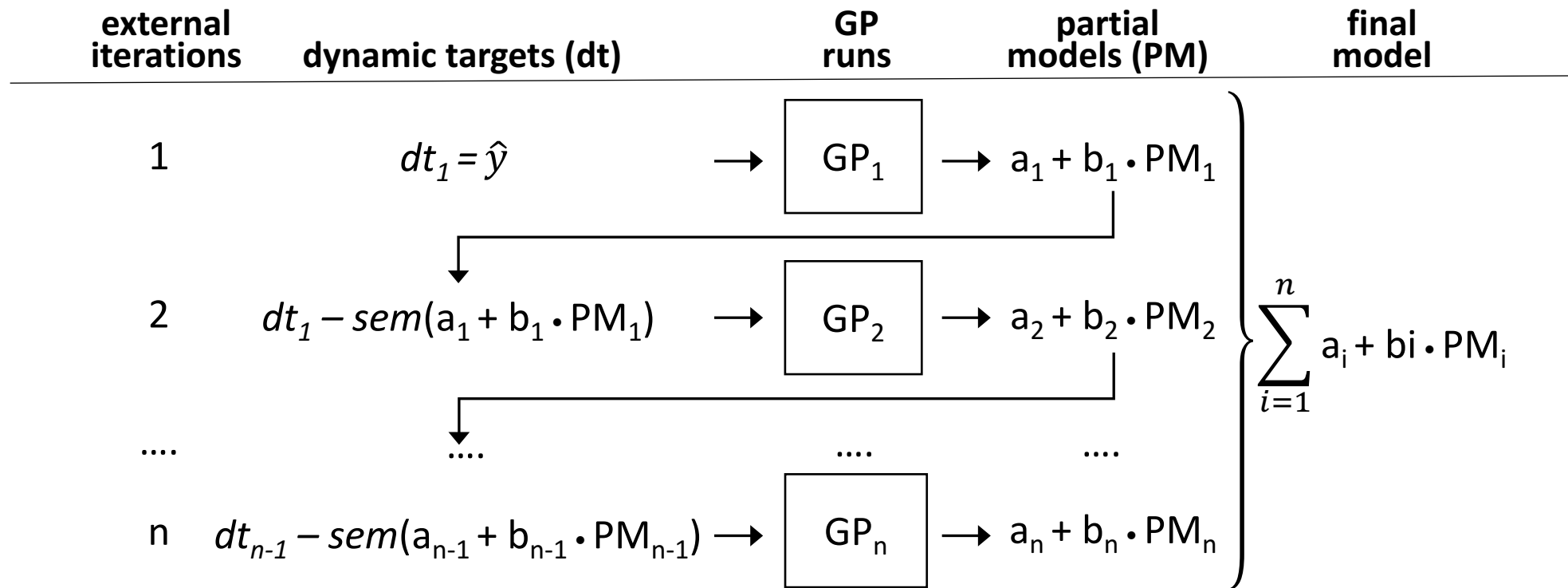
# SGP-DT: SGP Based on Dynamic Targets



# SGP-DT: SGP Based on Dynamic Targets

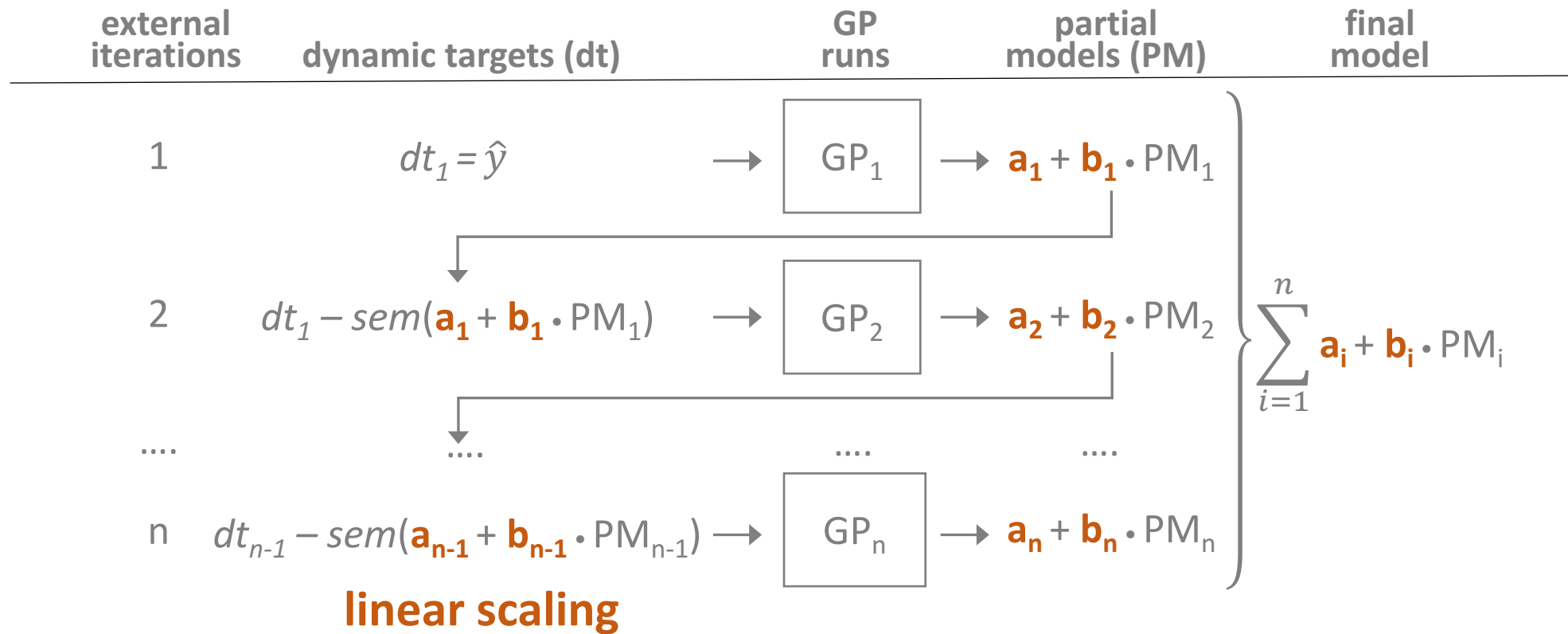


# SGP-DT: SGP Based on Dynamic Targets





# SGP-DT: SGP Based on Dynamic Targets



# Linear Scaling (Keijzer 2003)

$$\mathcal{I}_{ls} = a + b \cdot \mathcal{I}$$

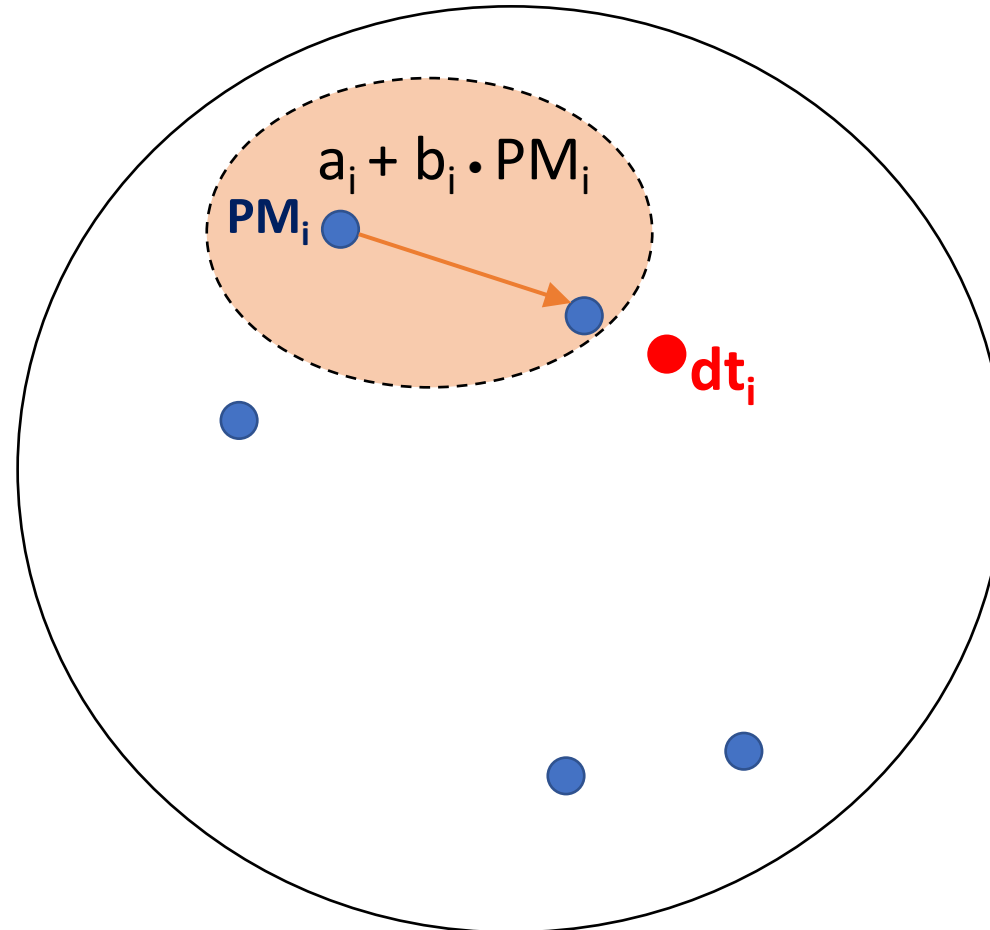
where  $a = \bar{\hat{y}} - b \cdot \bar{y}$  and  $b = \frac{\sum_{i=1}^n [(\hat{y}_i - \bar{\hat{y}}) \cdot (y_i - \bar{y})]}{\sum_{i=1}^n [(y_i - \bar{y})^2]}$

*intersect*                      *slope*

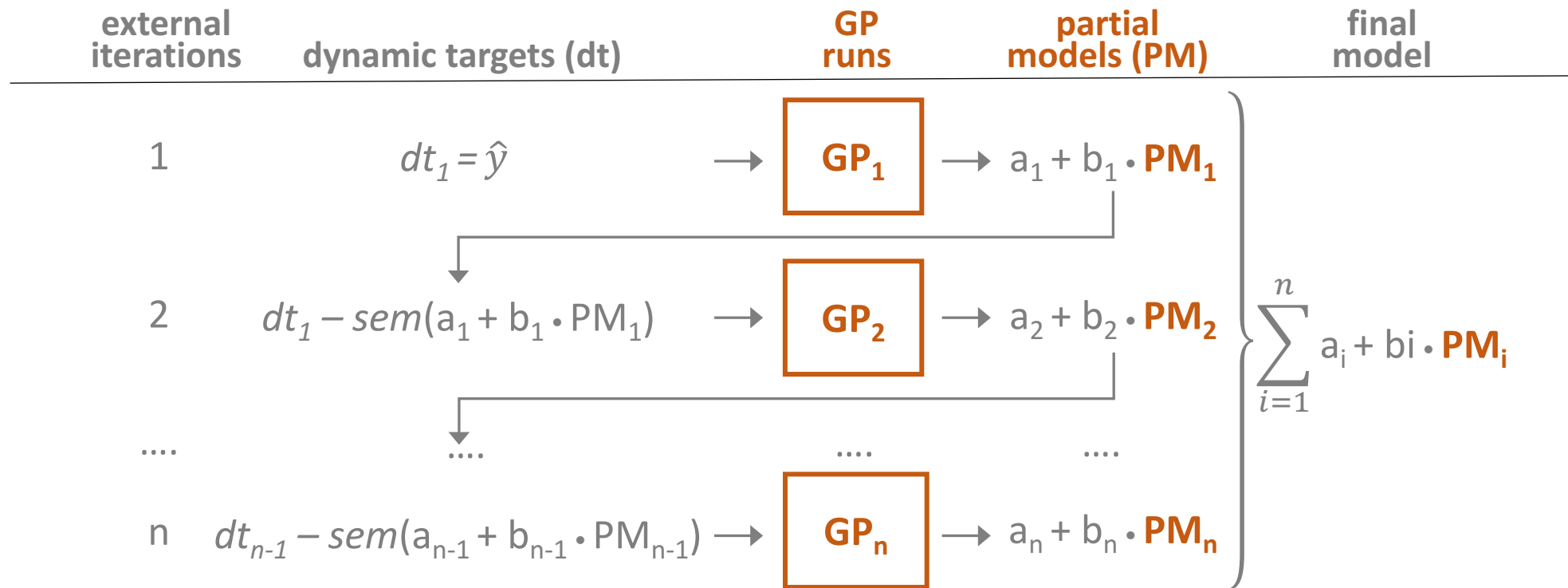
- it guarantees a bound on the error
- directly optimizes the model without waiting that GP spontaneously evolve it

# Linear Scaling (Keijzer 2003)

## (Semantic) Search Space



# SGP-DT: SGP Based on Dynamic Targets



# Individuals

Individual:

Tree-like expression

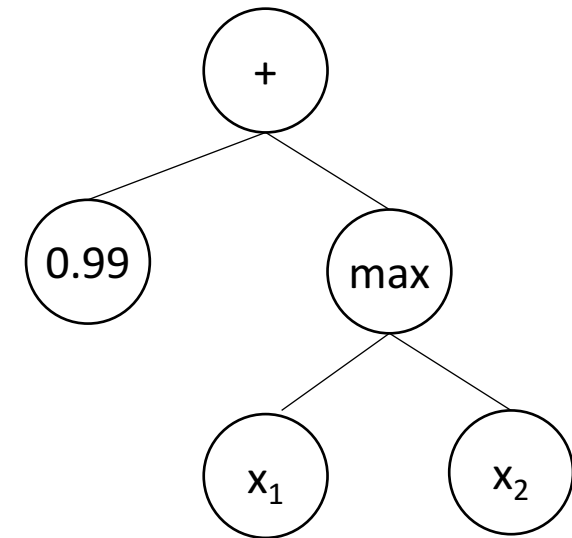
Symbols:

$+$ ,  $-$ ,  $x$ ,  $/$ , ERC  $[-1 ; +1]$ , Min and Max

Genetic operators:

Mutation: subtree substitution

Elite: one individual



# Fitness Function

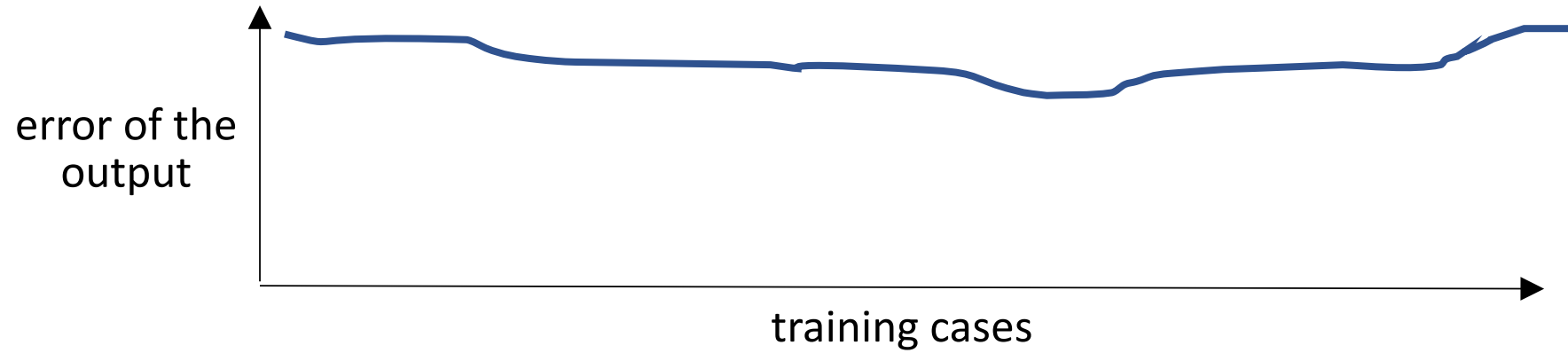
$$\text{error} = \text{sem}(a + b \cdot I) - \hat{y}$$

$$\text{Fitness-function}(I) = \sigma^2(\text{error})$$

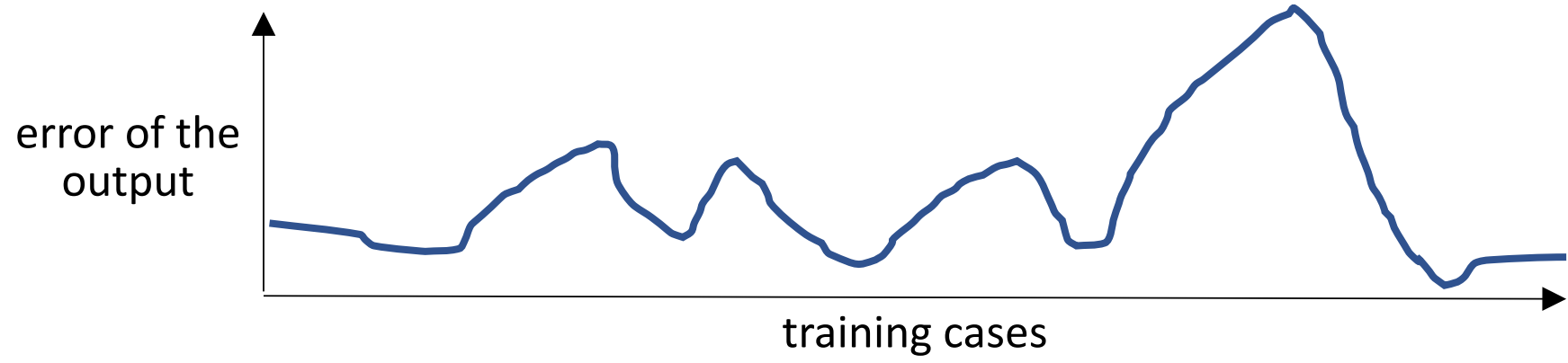
$$\text{MSE} = \frac{\sum_{i=0}^m (y_i - \hat{y}_i)^2}{m} \leq \sigma^2(\hat{y}) \quad \text{due to linear scaling}$$

$\sigma^2(\hat{y})$  is an upper bound on the MSE

# Fitness Function



*low  $\sigma^2$   
high error*



*high  $\sigma^2$   
low error*

# GP Runs

## Tournament Selection

We reduce the disruptiveness of GP operators by:

- Avoiding Crossover

- Only Mutation (biased towards the leaves)



# GP Runs

## Tournament Selection

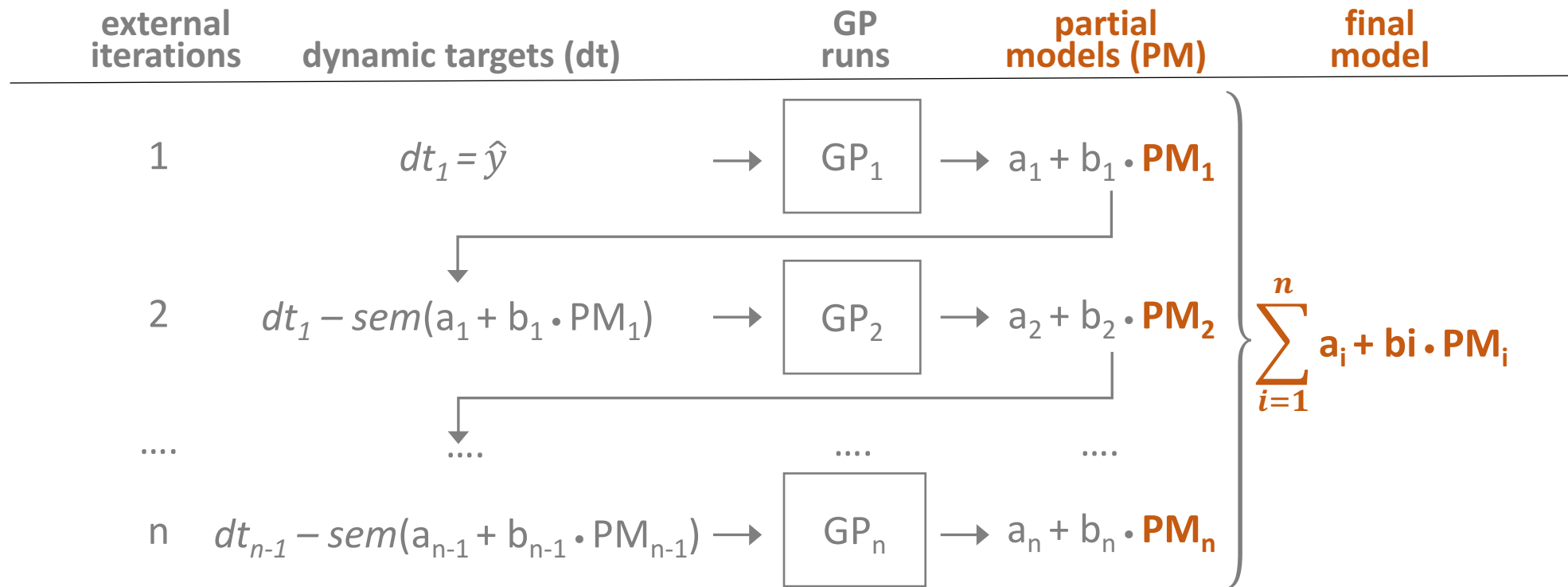
We reduce the disruptiveness of GP operators by:

Avoiding Crossover

Only Mutation (biased towards the leaves)

Without Crossover how SGP-DT exchanges genetic materials and functionalities?

# SGP-DT: SGP Based on Dynamic Targets



# Final Model

$$\sum_{i=1}^1 a_i + b_i \cdot PM_i$$



$$a_1 + b_1 \cdot PM_1$$

$$a_2 + b_2 \cdot PM_2$$

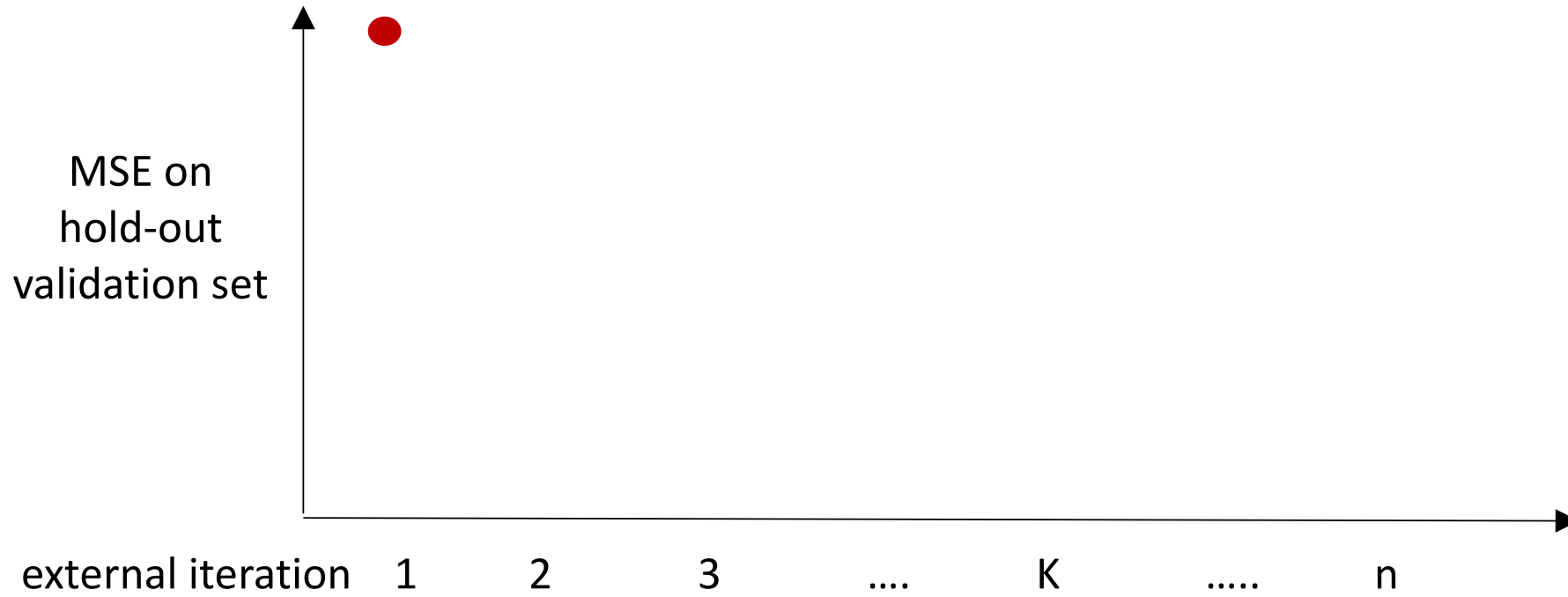
$$a_3 + b_3 \cdot PM_3$$

.....

$$a_K + b_K \cdot PM_K$$

.....

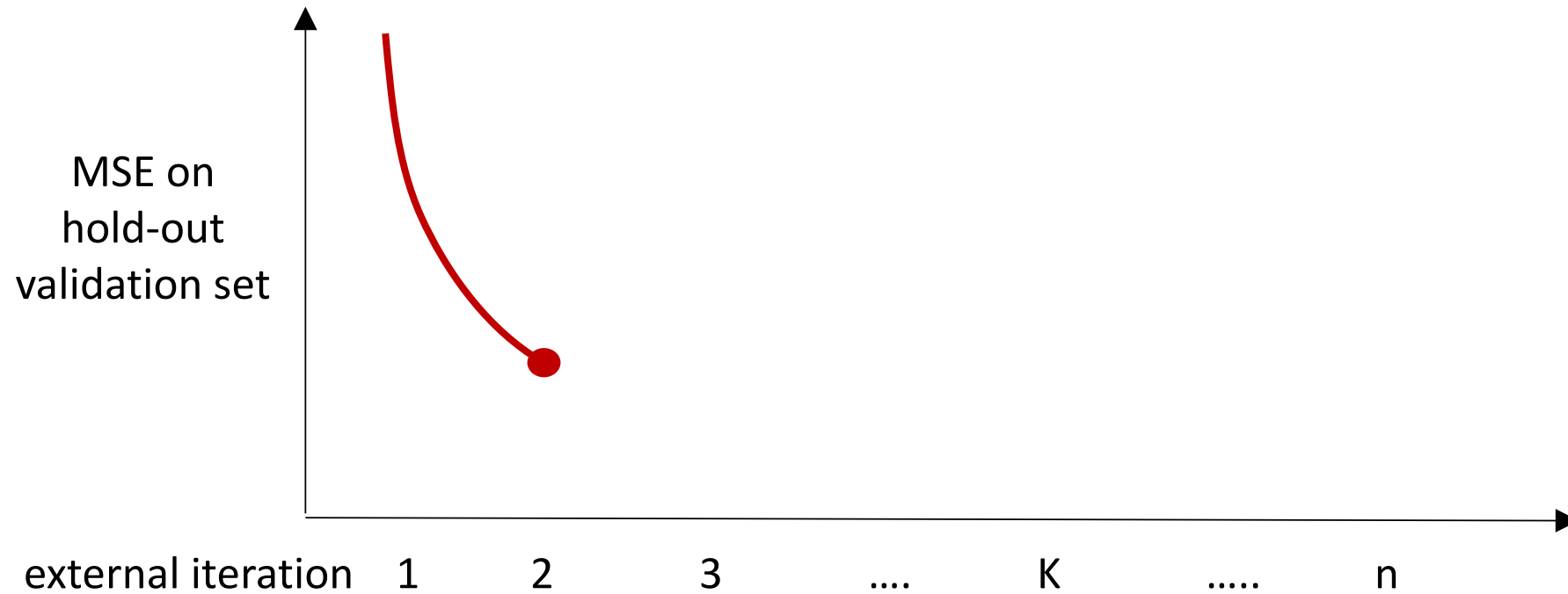
$$a_n + b_n \cdot PM_n$$



# Final Model

$$\sum_{i=1}^2 a_i + b_i \cdot PM_i$$

$a_1 + b_1 \cdot PM_1$     $a_2 + b_2 \cdot PM_2$     $a_3 + b_3 \cdot PM_3$    .....    $a_K + b_K \cdot PM_K$    .....    $a_n + b_n \cdot PM_n$

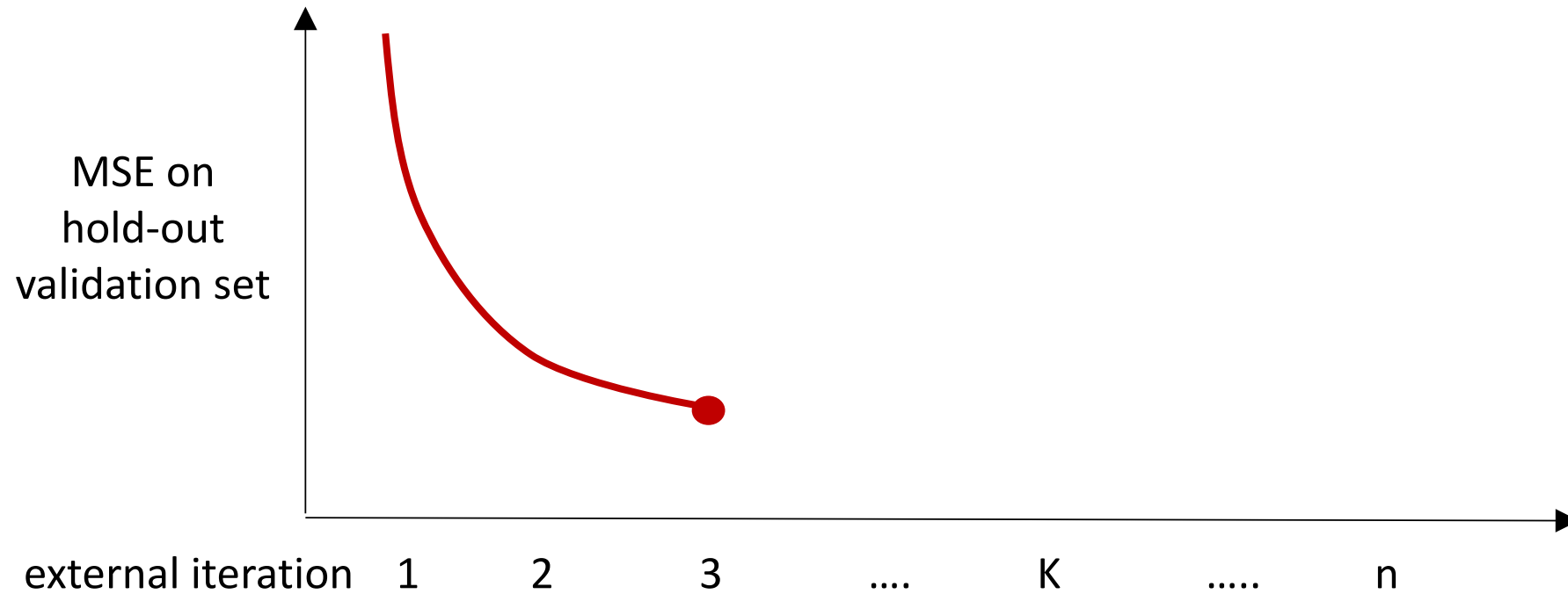


# Final Model

$$\sum_{i=1}^3 a_i + b_i \cdot PM_i$$

$a_1 + b_1 \cdot PM_1$     $a_2 + b_2 \cdot PM_2$     $a_3 + b_3 \cdot PM_3$    ....    $a_K + b_K \cdot PM_K$    ....    $a_n + b_n \cdot PM_n$

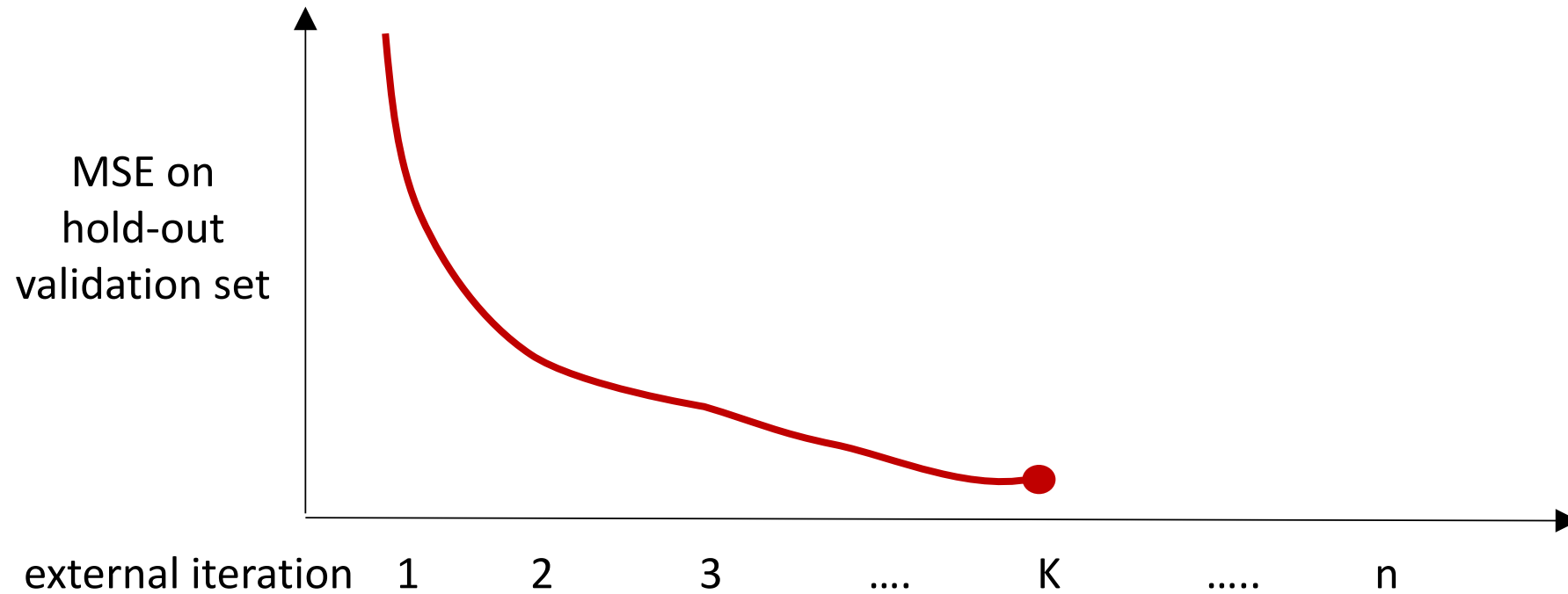
An upward-pointing arrow is positioned below the term  $a_3 + b_3 \cdot PM_3$ , pointing towards the summation symbol in the equation above.



# Final Model

$$a_1 + b_1 \cdot PM_1 \quad a_2 + b_2 \cdot PM_2 \quad a_3 + b_3 \cdot PM_3 \quad \dots \quad a_K + b_K \cdot PM_K \quad \dots \quad a_n + b_n \cdot PM_n$$
$$\sum_{i=1}^K a_i + b_i \cdot PM_i$$

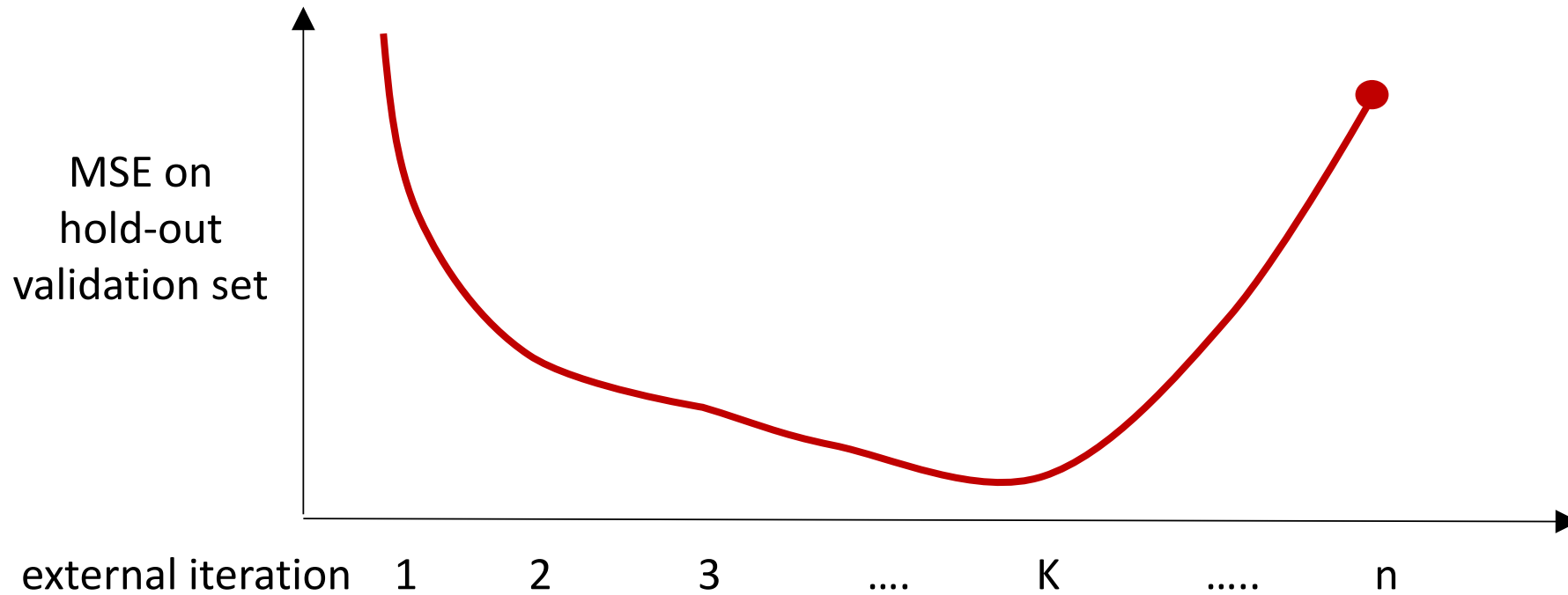
↑



# Final Model

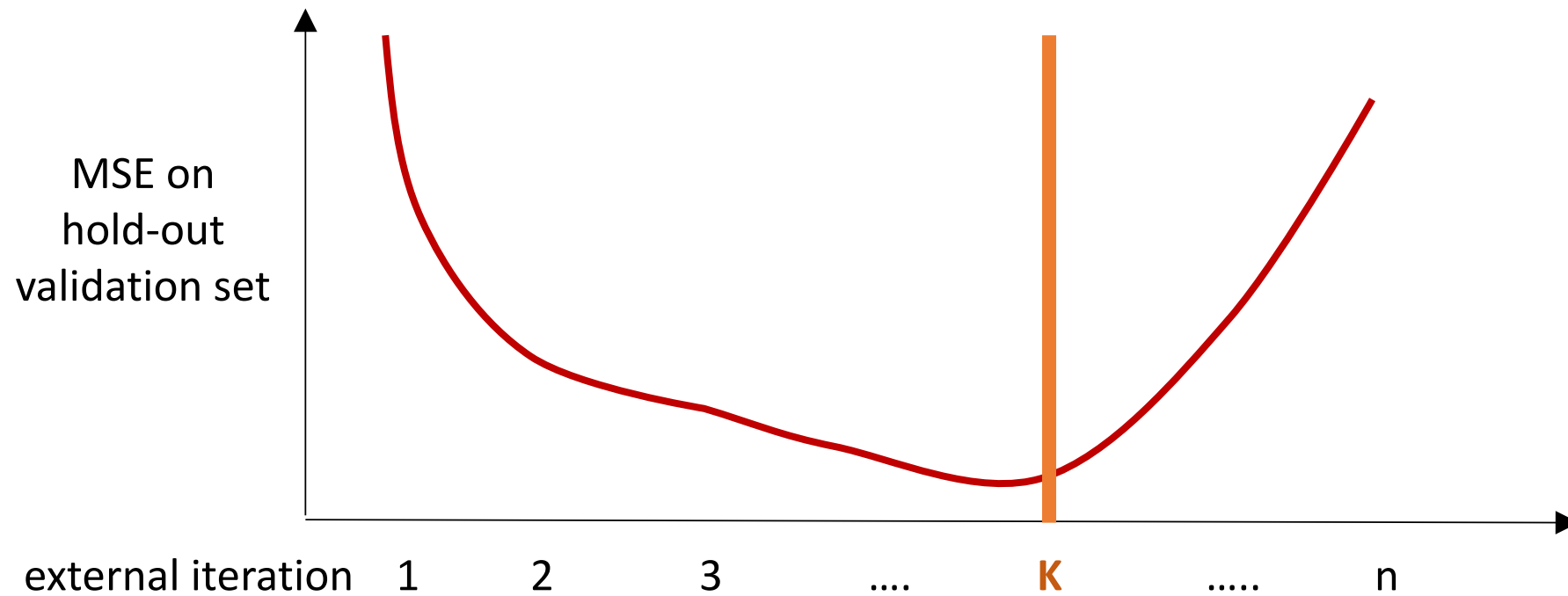
$$a_1 + b_1 \cdot PM_1 \quad a_2 + b_2 \cdot PM_2 \quad a_3 + b_3 \cdot PM_3 \quad \dots \quad a_K + b_K \cdot PM_K \quad \dots \quad a_n + b_n \cdot PM_n$$
$$\sum_{i=1}^K a_i + b_i \cdot PM_i$$

↑



# Final Model

$$a_1 + b_1 \cdot PM_1 \quad a_2 + b_2 \cdot PM_2 \quad a_3 + b_3 \cdot PM_3 \quad \dots \quad a_K + b_K \cdot PM_K \quad \dots \quad a_n + b_n \cdot PM_n$$
$$\sum_{i=1}^K a_i + b_i \cdot PM_i$$





Evaluation

# Subjects

name	# attributes	# instances
airfoil	5	1,503
concrete	8	1,030
enc	8	768
enh	8	768
housing	14	506
tower	25	3,135
yatch	6	309
uball5d	5	6,024

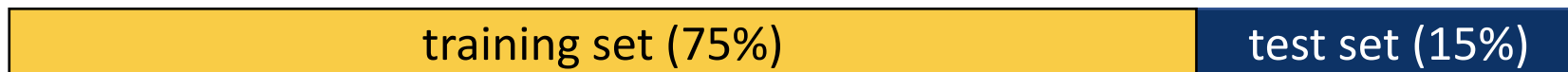


# Subjects

name	# attributes	# instances
airfoil	5	1,503
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housing	14	506
tower	25	3,135
yatch	6	309
uball5d	5	6,024



  
50 times

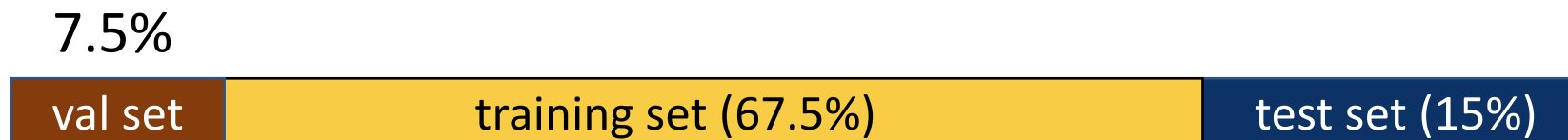


# Subjects

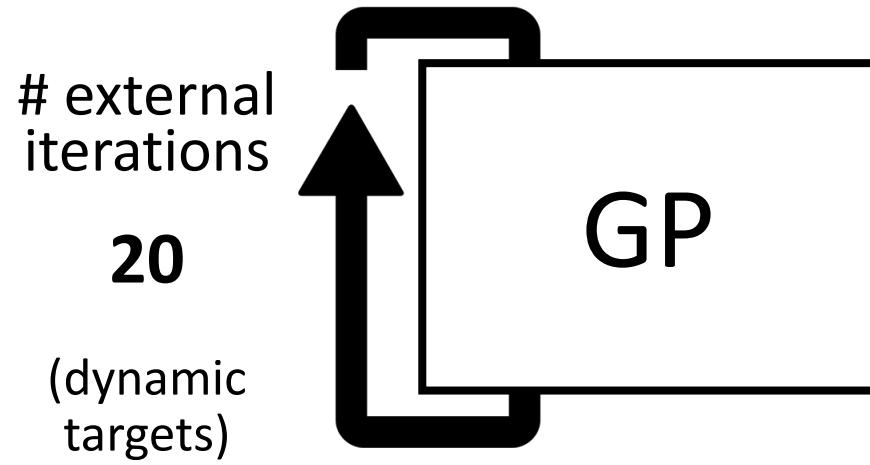
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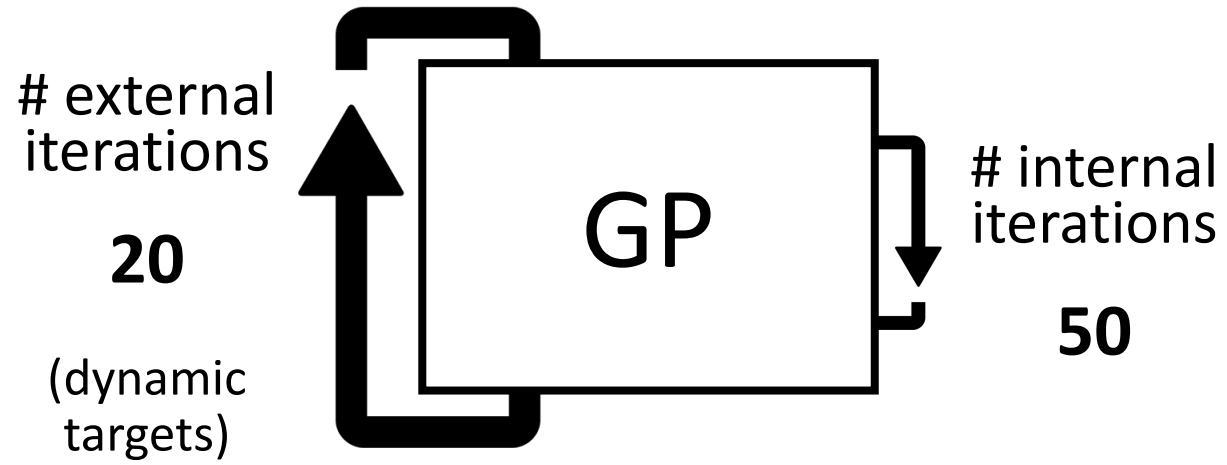
  
50 times



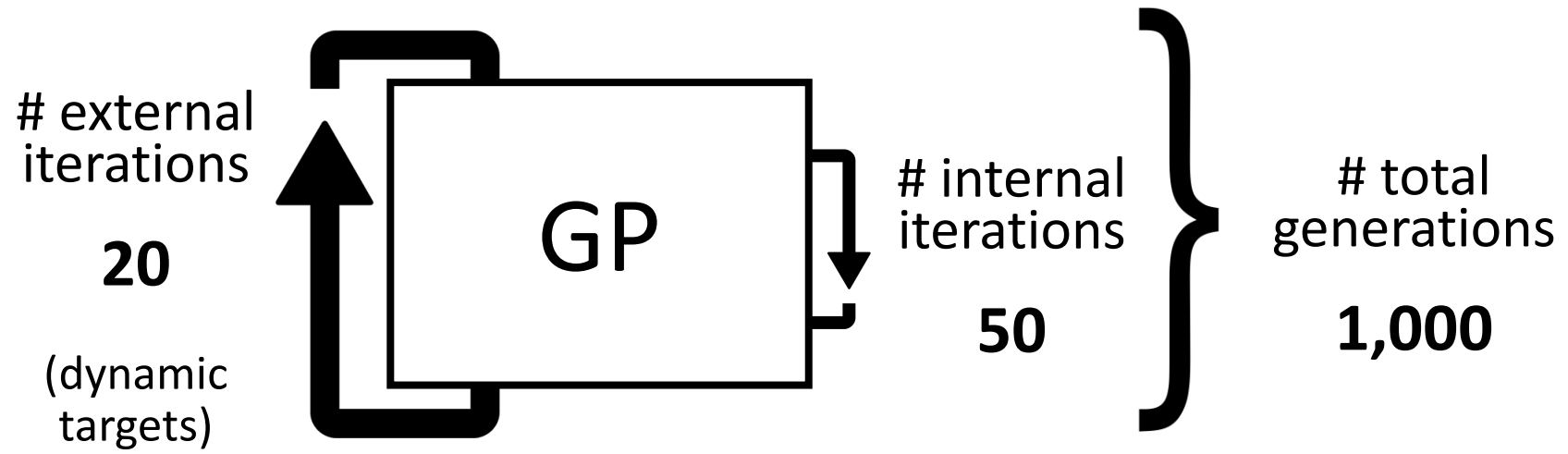
# SGP-DT Evaluation Setup



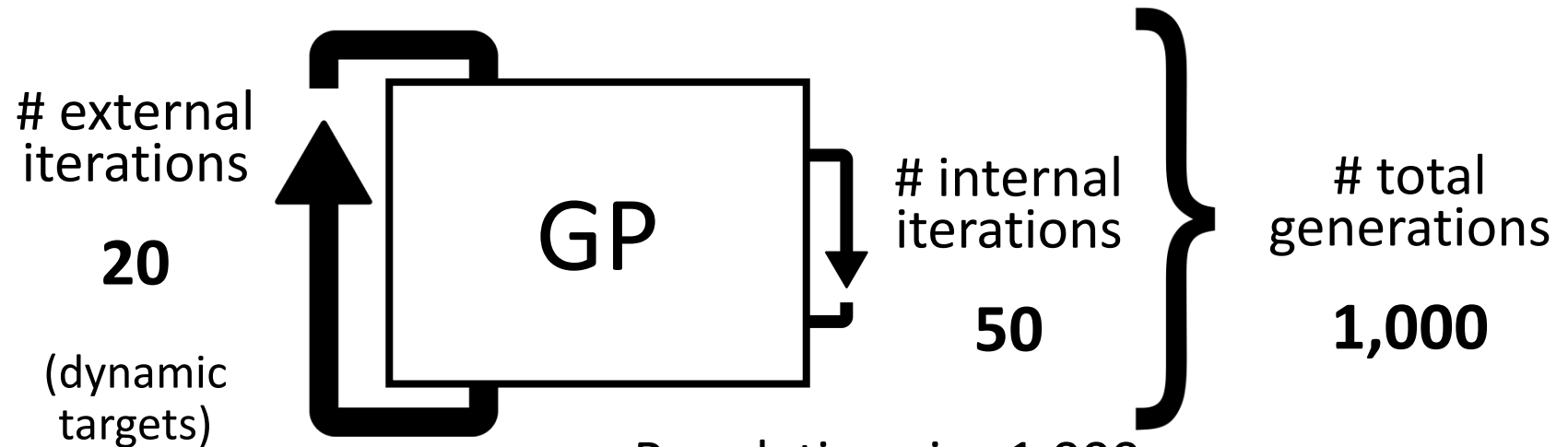
# SGP-DT Evaluation Setup



# SGP-DT Evaluation Setup



# SGP-DT Evaluation Setup



- Population size 1,000
- Probability mutation 100%
- Size elitism 1
- No bound on the size of the individuals



# Results (median RMSE 50 trials)

Median Root Mean Square Error (RMSE)	
subject	SGP-DT
airfoil	2.46
concrete	6.51
enc	1.48
enh	.56
housing	4.47
tower	.26
yatch	1.02
uball5d	.04

# Competitors

## **Lasso** (Efron 2004)

Least square regression method

## **$\epsilon$ -lexicase** (La Cava 2016)

Evolutionary technique based on lexicase (Starosta 70s)

Outperforms many GP algorithms

We ran 1,000 generations (same as SGP-DT)

Validation set (10% of the training set)

# Results (median RMSE 50 trials)


subject	Median Root Mean Square Error (RMSE)		
	SGP-DT	Lasso	$\epsilon$ -lexicase
airfoil	2.46	4.85	3.65
concrete	6.51	10.54	7.07
enc	1.48	3.25	1.86
enh	.56	2.96	1.29
housing	4.47	4.91	4.28
tower	.26	.29	.30
yatch	1.02	9.02	1.36
uball5d	.04	.19	.06

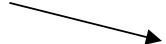
# Results (median RMSE 50 trials)

subject	Median Root Mean Square Error (RMSE)		
	SGP-DT	Lasso	$\epsilon$ -lexicase
airfoil	2.46	4.85	3.65
concrete	6.51	10.54	7.07
enc	1.48	3.25	1.86
enh	.56	2.96	1.29
housing	4.47	4.91	4.28
tower	.26	.29	.30
yatch	1.02	9.02	1.36
uball5d	.04	.19	.06

# Results (median RMSE 50 trials)

subject	Median Root Mean Square Error (RMSE)		
	SGP-DT	Lasso	$\epsilon$ -lexicase
airfoil	2.46	+49%	+32%
concrete	6.51	+38%	+8%
enc	1.48	+54%	+20%
enh	.56	+81%	+57%
housing	4.47	+9%	-4%
tower	.26	+12%	+12%
yatch	1.02	+89%	+25%
uball5d	.04	+79%	+35%

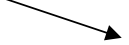

$$\frac{\text{Lasso} - \text{SGP-DT}}{\text{Lasso}} \cdot 100$$


$$\frac{\epsilon\text{-lexicase} - \text{SGP-DT}}{\epsilon\text{-lexicase}} \cdot 100$$

# SGP-DT Variants

**DT-EM** Directly minimize the error

$$\textit{Fitness-function (I)} = \text{MSE} = \frac{\sum_{i=0}^m (y_i - \hat{y}_i)^2}{m}$$

$m$    
# training cases

**DT-NM** without Min and Max

+, -, x, /

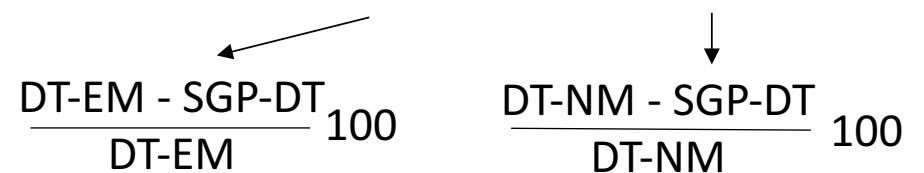
ERC [-1; +1]

~~Min Max~~

# Results (median RMSE 50 trials)

subject	Median Root Mean Square Error (RMSE)		
	SGP-DT	DT-EM	DT-NM
airfoil	2.46	+4%	+16%
concrete	6.51	-1%	-2%
enc	1.48	+1%	-2%
enh	.56	+3%	-3%
housing	4.47	-1%	+1%
tower	.26	+10%	+10%
yatch	1.02	+20%	+13%
uball5d	.04	+7%	-8%

$\frac{DT-EM - SGP-DT}{DT-EM} \cdot 100$        $\frac{DT-NM - SGP-DT}{DT-NM} \cdot 100$



# Results (number of evaluated nodes 50 trials)

<b>subject</b>	<b>Median Number of Evaluated Nodes</b>
	<b>SGP-DT</b>
airfoil	1.00E+10
concrete	1.14E+10
enc	1.18E+10
enh	1.18E+10
housing	7.70E+09
tower	7.21E+10
yatch	4.62E+09
uball5d	9.83E+10



# Results (number of evaluated nodes 50 trials)

subject	Median Number of Evaluated Nodes			
	SGP-DT	$\epsilon$ -lexicase	DT-EM	DT-NM
airfoil	1.00E+10	9.26x	1.00x	.90x
concrete	1.14E+10	5.64x	1.00x	.77x
enc	1.18E+10	4.25x	.99x	.80x
enh	1.18E+10	4.30x	.99x	.78x
housing	7.70E+09	4.02x	.99x	.78x
tower	7.21E+10	2.69x	.99x	.62x
yatch	4.62E+09	4.34x	.99x	.75x
uball5d	9.83E+10	4.01x	.99x	.76x

↓

$\frac{\epsilon\text{-lexicase}}{\text{SGP-DT}}$

↓

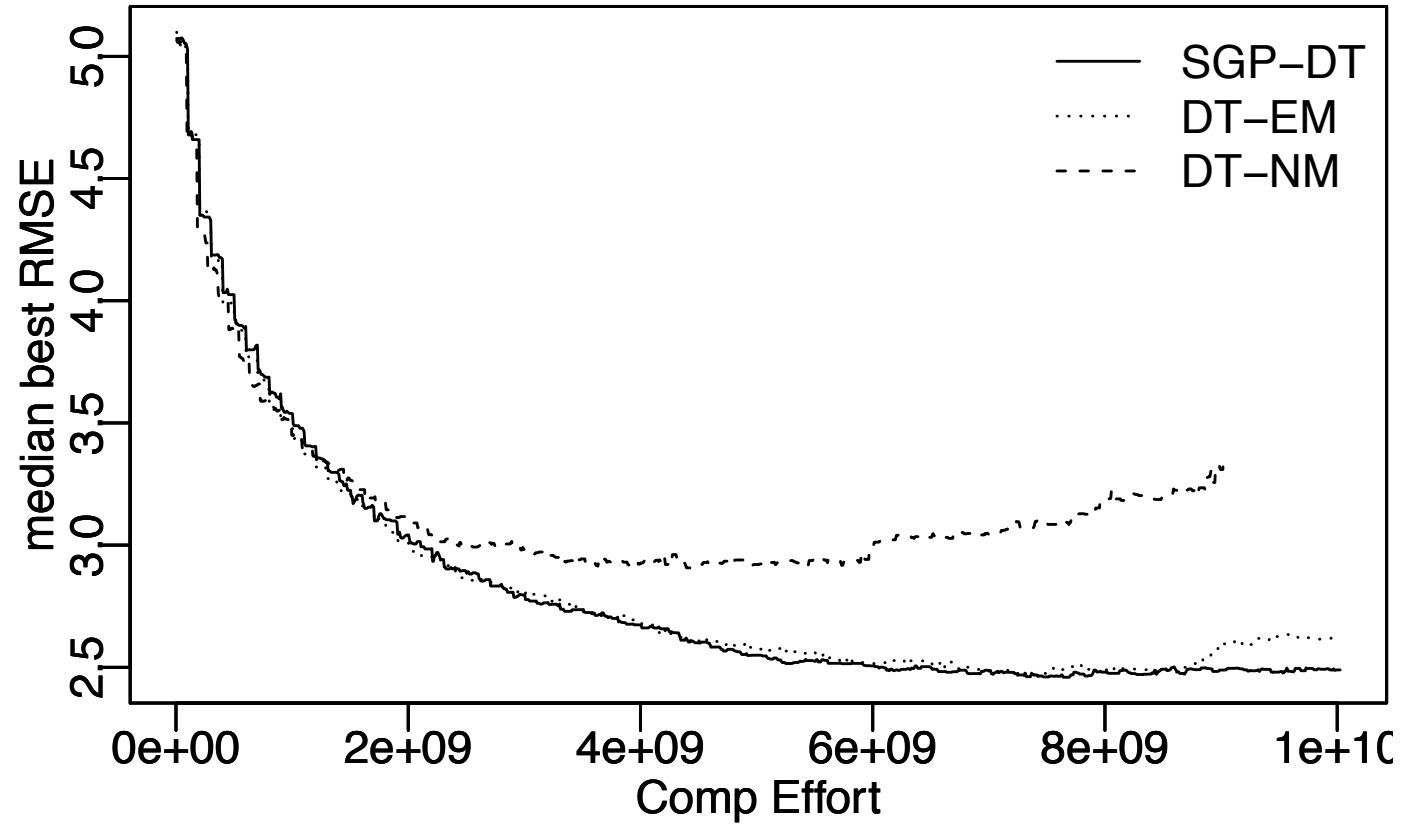
$\frac{\text{DT-EM}}{\text{SGP-DT}}$

↓

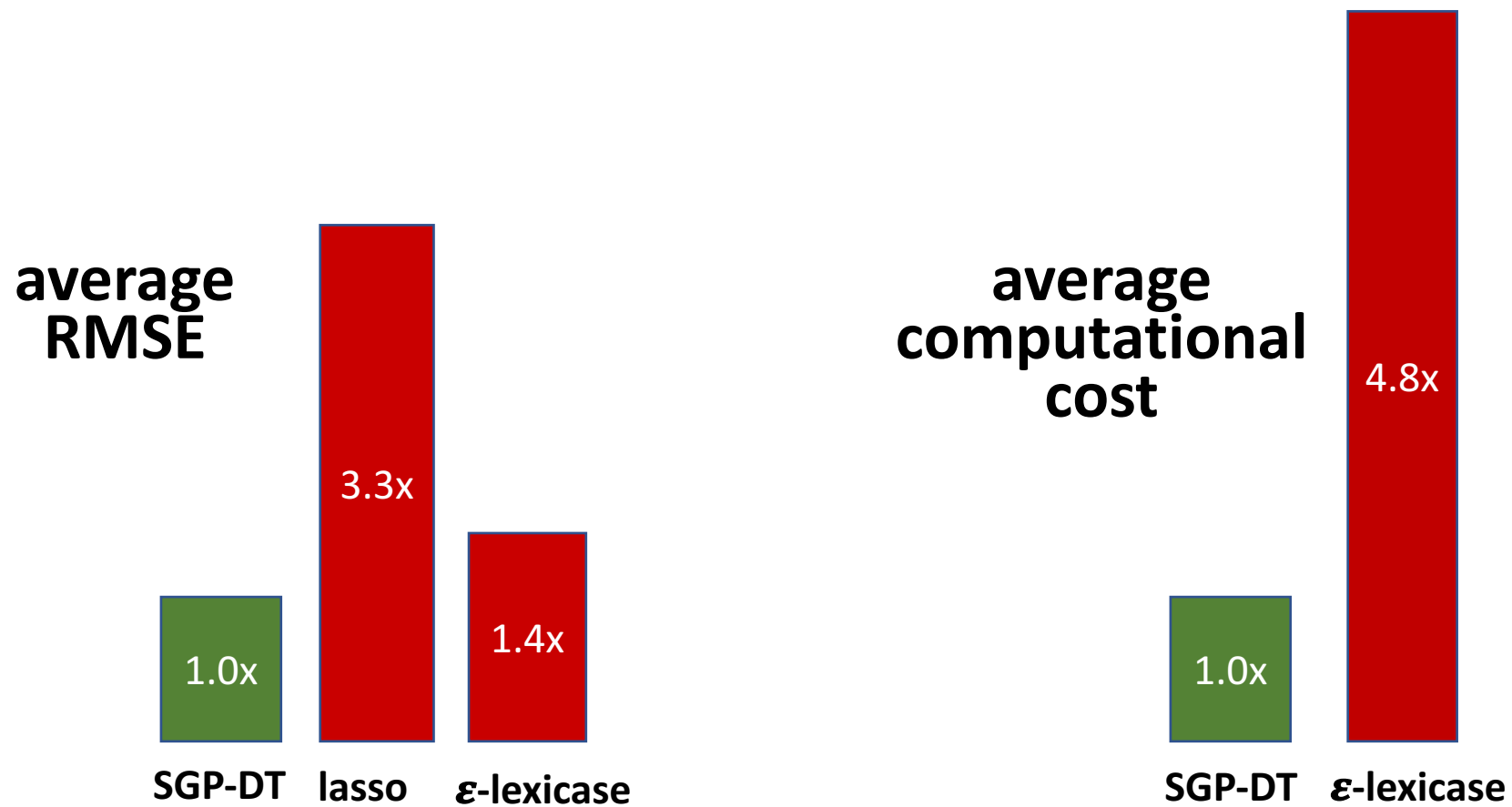
$\frac{\text{DT-NM}}{\text{SGP-DT}}$

# Overfitting

airfoil dataset



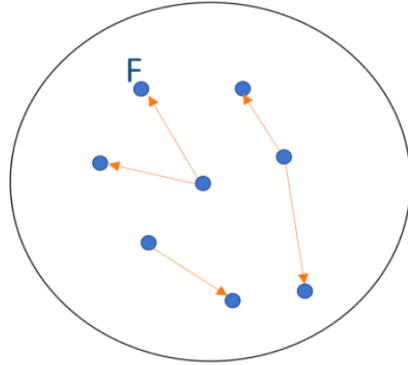
# Results Summary



# Conclusion

Semantic Genetic Programming (SGP)

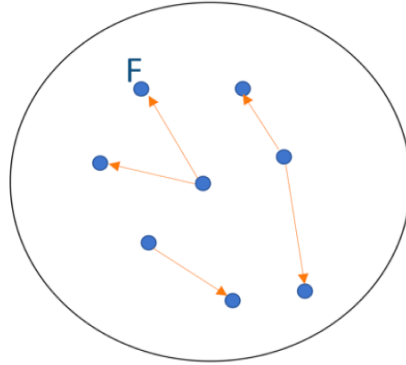
**(Semantic) Search Space**



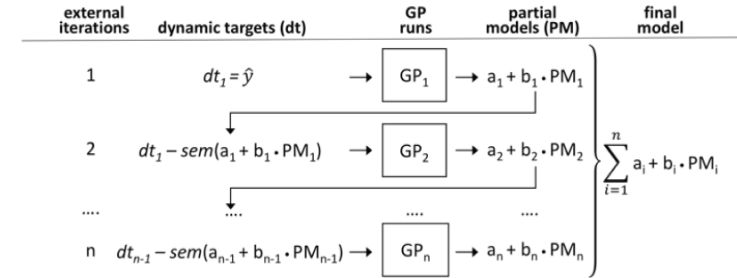
# Conclusion

## Semantic Genetic Programming (SGP)

(Semantic) Search Space



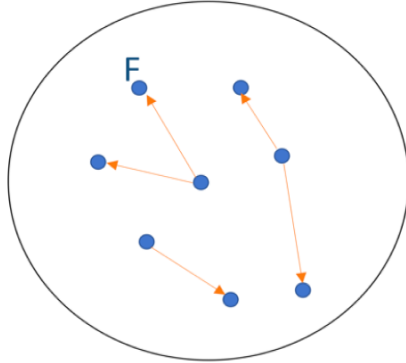
## SGP-DT: SGP Based on Dynamic Targets



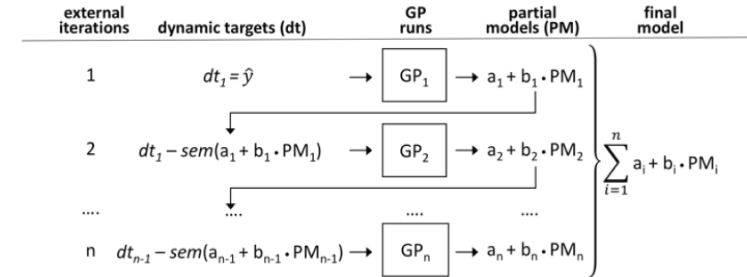
# Conclusion

## Semantic Genetic Programming (SGP)

(Semantic) Search Space



## SGP-DT: SGP Based on Dynamic Targets



## Subjects

name	# attributes	# instances
airfoil	5	1,503
concrete	8	1,030
enc	8	768
enh	8	768
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tower	25	3,135
yacht	6	309
uball5d	5	6,024



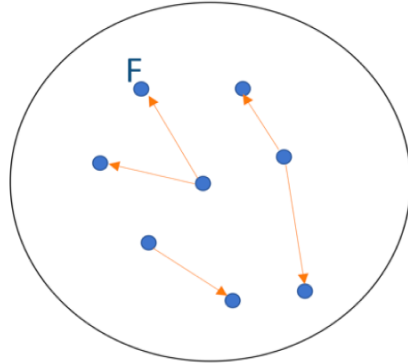
50 times



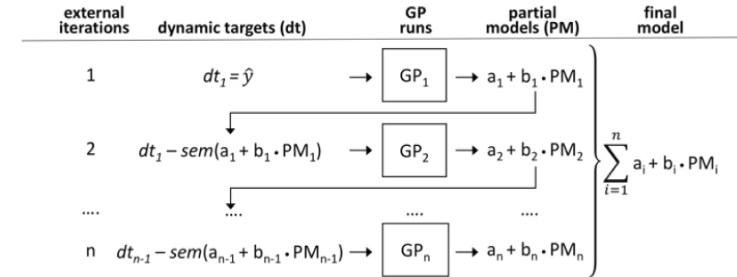
# Conclusion

## Semantic Genetic Programming (SGP)

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## SGP-DT: SGP Based on Dynamic Targets



## Subjects

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housing	14	506
tower	25	3,135
yacht	6	309
uball5d	5	6,024



50 times



## Results (median RMSE 50 trials)

subject	Median Root Mean Square Error (RMSE)				
	SGP-DT	Lasso	$\epsilon$ -lexicase	DT-EM	DT-NM
airfoil	2.46	+49%	+32%	+4%	+16%
concrete	6.51	+38%	+8%	-1%	-2%
enc	1.48	+54%	+20%	+1%	-2%
enh	.56	+81%	+57%	+3%	-3%
housing	4.47	+9%	-4%	-1%	+1%
tower	.26	+12%	+12%	+10%	+10%
yacht	1.02	+89%	+25%	+20%	+13%
uball5d	.04	+79%	+35%	+7%	-8%

# Conclusion

Semantic Genetic Programming (SGP)

(Semantic) Search Space

SGP-DT: SGP Based on Dynamic Targets

## Future Work

- 1 semantically-aware minimization
- 2 filtering partial models
- 3 self-adapting hyper-parameters
- 4 classification problem

$$\begin{array}{l}
 \text{external} \quad \text{GP} \quad \text{partial} \quad \text{final} \\
 \text{models (PM)} \quad \text{model} \\
 \left. \begin{array}{l}
 b_1 \cdot PM_1 \\
 b_2 \cdot PM_2 \\
 \dots \\
 b_n \cdot PM_n
 \end{array} \right\} \sum_{i=1}^n a_i + b_i \cdot PM_i
 \end{array}$$

name	# attr
airfoil	
concrete	
enc	
enh	
housing	
tower	25
yacht	6
uball5d	5

	3,135
	309
	6,024

50 times



trials)

(RMSE)	
DT-EM	DT-NM
+4%	+16%
-1%	-2%
+1%	-2%
+3%	-3%
-1%	+1%
+10%	+10%
+20%	+13%
+7%	-8%

enh	.56	+81%	+57%	+3%	-3%
housing	4.47	+9%	-4%	-1%	+1%
tower	.26	+12%	+12%	+10%	+10%
yacht	1.02	+89%	+25%	+20%	+13%
uball5d	.04	+79%	+35%	+7%	-8%



# Results (median RMSE)

subject	Median Root Mean Square Error (RMSE)				
	SGP-DT	Lasso	$\epsilon$ -lexicase	DT-EM	DT-NM
airfoil	2.4634	4.8484	3.6505	2.5643	2.9237
concrete	6.5123	10.5383	7.0707	6.4476	6.4132
enc	1.4838	3.2498	1.8647	1.4993	1.4584
enh	0.5560	2.9645	1.2952	0.5714	0.5410
housing	4.4700	4.9155	4.2785	4.4377	4.5273
tower	0.2606	0.2953	0.2975	0.2900	0.2900
yacht	1.0221	9.0237	1.3577	1.2849	0.0372
uball5d	0.0402	0.1939	0.0618	0.0430	1.1786