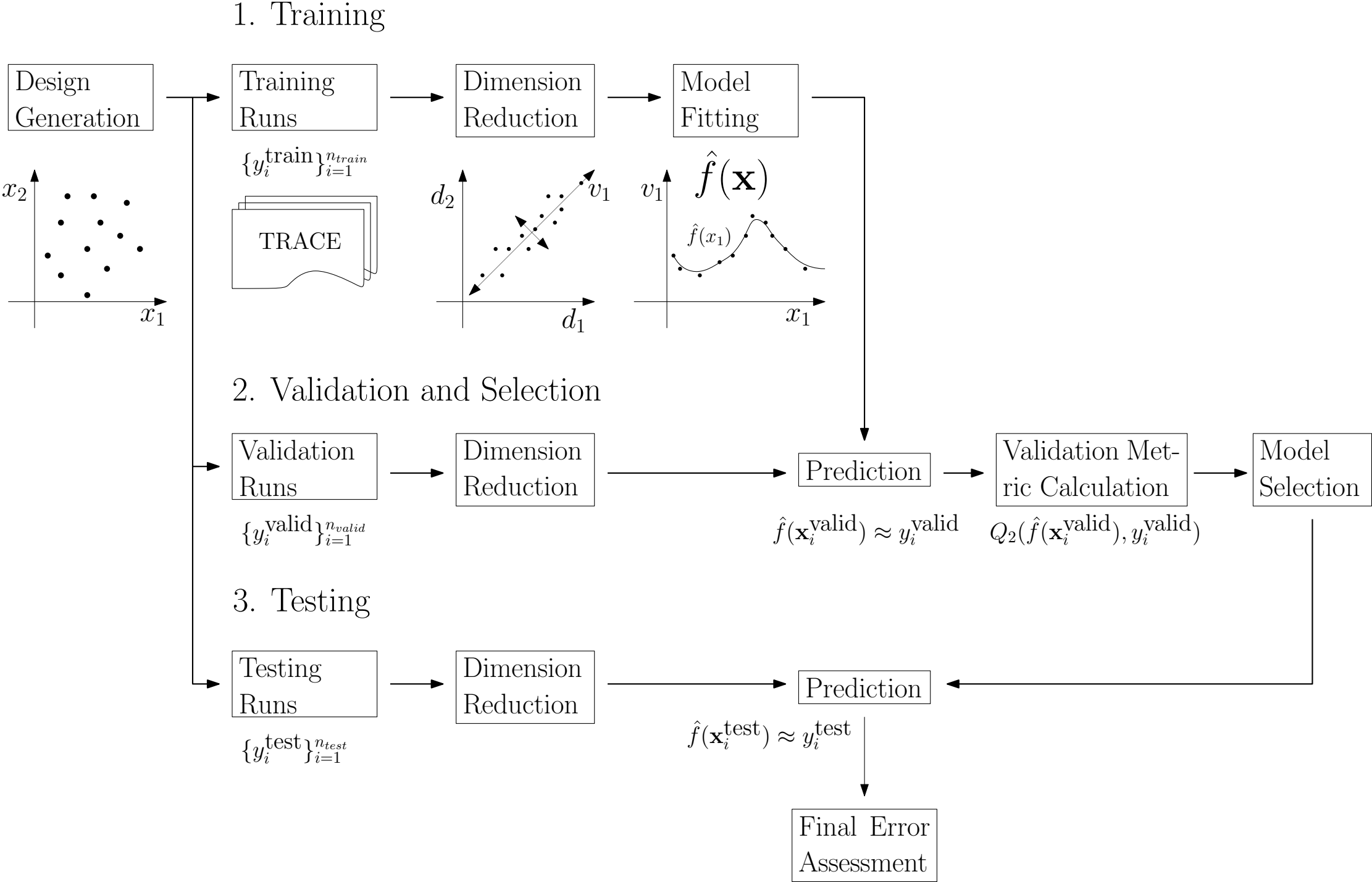
1. Training
Design Generation
Training Runs
Dimension Reduction
Model Fitting
$\{y_i^{\text{train}}\}_{i=1}^{n_{train}}$
TRACE
x_2
x_1
d_2
v_1
d_1
v_1
$\hat{f}(\mathbf{x})$
$\hat{f}(x_1)$
x_1
2. Validation and Selection
Validation Runs
Dimension Reduction
Prediction
Validation Metric Calculation
Model Selection
$\{y_i^{\text{valid}}\}_{i=1}^{n_{valid}}$
$\hat{f}(\mathbf{x}_i^{\text{valid}}) \approx y_i^{\text{valid}}$
$Q_2(\hat{f}(\mathbf{x}_i^{\text{valid}}), y_i^{\text{valid}})$
3. Testing
Testing Runs
Dimension Reduction
Prediction
$\{y_i^{\text{test}}\}_{i=1}^{n_{test}}$
$\hat{f}(\mathbf{x}_i^{\text{test}}) \approx y_i^{\text{test}}$
Final Error Assessment