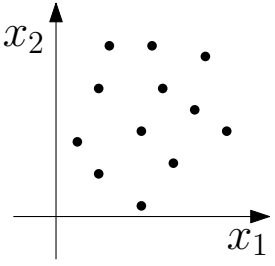
1. Training

Design Generation



$\{\mathbf{x}_i^{\text{train}}\}_{i=1}^{n_{train}}$

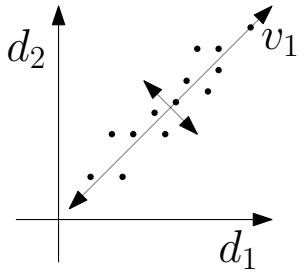
$\{\mathbf{x}_i^{\text{valid}}\}_{i=1}^{n_{valid}}$

$\{\mathbf{x}_i^{\text{test}}\}_{i=1}^{n_{test}}$

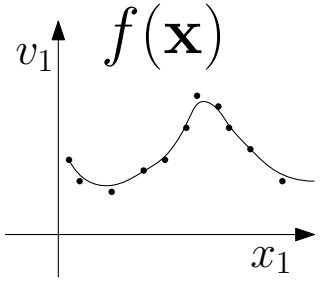
Training Runs

$\{\mathbf{y}_i^{\text{train}}\}_{i=1}^{n_{train}}$

Dimension Reduction



Model Fitting



2. Validation and Selection

Validation Runs

$\{\mathbf{y}_i^{\text{valid}}\}_{i=1}^{n_{valid}}$

Dimension Reduction

Prediction

$\hat{f}(\mathbf{x}_i^{\text{valid}}) \approx y_i^{\text{valid}}$

Validation Metric Calculation

$Q_2(\hat{f}(\mathbf{x}_i^{\text{valid}}), y_i^{\text{valid}})$

3. Testing

Testing Runs

$\{\mathbf{y}_i^{\text{test}}\}_{i=1}^{n_{test}}$

Dimension Reduction

Prediction

$\hat{f}(\mathbf{x}_i^{\text{test}}) \approx y_i^{\text{test}}$

Final Error Assessment