Lecture 10: Validation in Simulation

Simulation and Modeling Course

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1. Introduction

Validation is a critical step in the simulation modeling process. After a model is conceptually designed, mathematically formulated, and implemented using software, we need to ensure that the model **represents the real-world system accurately**. Validation evaluates whether the simulation output is realistic, consistent, and reliable.

Validation answers an essential question:

> *"Does the model behave like the real system it is intended to represent?"*

A model that is not validated may lead to incorrect decisions, misleading predictions, and unreliable conclusions especially in medical, engineering, and financial simulations.

Objectives of This Lecture

- Understand the concept and purpose of validation.
- Learn the difference between verification and validation.
- Explore different types of validation.
- Apply validation techniques to real examples.
- Discuss quantitative measures such as RMSE, MAPE, correlation, and R^2.
- Present a complete case study with implementation.

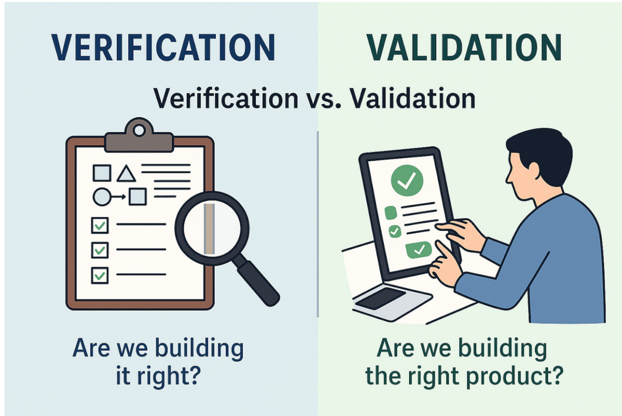

Figure 1: Conceptual distinction between verification and validation (placeholder).

2. Verification vs. Validation

Although often confused, these two steps are fundamentally different:

- **Verification**: Ensuring the model is implemented correctly ("Did we build the model right?").
- **Validation**: Ensuring the model accurately represents reality ("Did we build the right model?").

Verification is internal (correct implementation), while validation is external (comparison with real data or expert knowledge).

3. Types of Validation

Validation can be classified into several forms depending on the stage and available information.

3.1 Conceptual Model Validation

Ensures the logical structure of the model makes sense before coding. Includes:

- Checking assumptions.
- Reviewing flowcharts.
- Ensuring consistency with scientific theory.

3.2 Data Validation

Ensures input data are:

- Accurate,
- Clean,
- Representative of the real-world system.

3.3 Operational Validation

The most important type: comparing simulation results with real system performance.

Approaches include:

- Visualization comparison.
- Statistical hypothesis testing.
- Goodness-of-fit measures.
- Expert-based review.

3.4 Sensitivity-Based Validation

A model that changes drastically with small input variations is questionable. Stability indicates reliability.

4. Why Validation Is Important

- Ensures trustworthiness of model predictions.
- Supports decision-making in medicine, engineering, business, etc.
- Detects unrealistic assumptions.
- Reduces risk in complex simulations (drug dosing, ICU decisions, surgery planning).

In medical simulation, validation is essential because incorrect models may lead to dangerous clinical decisions.

5. Quantitative Validation Techniques

Assume we have real observations y_i and simulated outputs $\hat{y}_i$ for $i = 1, \ldots, n$.

5.1 Error Metrics

Mean Squared Error (MSE)

$$\text{MSE} = \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

Root Mean Squared Error (RMSE)

$$\text{RMSE} = \sqrt{\text{MSE}} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2}$$

Mean Absolute Percentage Error (MAPE)

$$\text{MAPE} = \frac{100}{n} \sum_{i=1}^{n} \left| \frac{y_i - \hat{y}_i}{y_i} \right|$$

5.2 Correlation

Correlation coefficient between real and simulated values:

$$r = \frac{\sum_{i=1}^{n} (y_i - \bar{y})(\hat{y}_i - \bar{\hat{y}})}{\sqrt{\sum_{i=1}^{n} (y_i - \bar{y})^2} \sqrt{\sum_{i=1}^{n} (\hat{y}_i - \bar{\hat{y}})^2}}$$

Values close to $r = 1$ indicate strong agreement.

5.3 Coefficient of Determination (R^2)

The coefficient of determination measures the proportion of variance in the real data explained by the model:

$$R^2 = 1 - \frac{\sum_{i=1}^{n} (y_i - \hat{y}_i)^2}{\sum_{i=1}^{n} (y_i - \bar{y})^2}$$

Values near $R^2 = 1$ correspond to a highly validated model.

5.4 Bias Metric

Sometimes we want to know if the model systematically overestimates or underestimates:

$$\text{Bias} = \frac{1}{n}\sum_{i=1}^{n}(\hat{y}_i - y_i)$$

A bias close to zero indicates no systematic over- or underestimation.

5.5 Hypothesis Testing

Examples:

- Chi-square goodness-of-fit test.
- Kolmogorov–Smirnov test.
- Paired t-test for comparing mean outputs.

6. Example 1: Validating a Queue Simulation (Hospital ED)

Consider a hospital emergency department (ED). We focus on the **average waiting time** W as a key performance metric.

6.1 Real vs. Simulated Metrics

Let:

$$W_{\text{real}} = 28 \text{ minutes}, \qquad W_{\text{sim}} = 31 \text{ minutes}$$

We define the **absolute error** in waiting time:

$$\text{AE}_W = |W_{\text{sim}} - W_{\text{real}}| = |31 - 28| = 3 \text{ minutes}$$

The **relative error** (percentage error) is:

$$\text{RE}_W = \left|\frac{W_{\text{sim}} - W_{\text{real}}}{W_{\text{real}}}\right| \times 100 = \left|\frac{31 - 28}{28}\right| \times 100 \approx 10.7\%$$

If the acceptable validation threshold is, for example, 15%, the model is considered valid for this metric.

7. Example 2: Drug Concentration Model Validation

Assume a patient receives a medication and the true concentration in blood is measured at four time points. We compare:

$$C_{\text{real}}(t) = \{10, 7.5, 5.2, 3.1\}, \qquad C_{\text{sim}}(t) = \{9.4, 7.0, 5.9, 3.4\}$$

7.1 RMSE for Drug Concentration

$$\text{MSE} = \frac{(10-9.4)^2 + (7.5-7.0)^2 + (5.2-5.9)^2 + (3.1-3.4)^2}{4}$$

$$\text{MSE} = \frac{0.36 + 0.25 + 0.49 + 0.09}{4} = 0.2975$$

$$\text{RMSE} = \sqrt{0.2975} \approx 0.545$$

A small RMSE indicates strong agreement between the model and the real system.

7.2 Area Under the Curve (AUC) Metric

In pharmacokinetics, a key metric is the **area under the curve** (AUC) of concentration vs. time, which represents total drug exposure.

Using the trapezoidal rule for times $t_1 < t_2 < \cdots < t_n$ and concentrations $C(t_i)$:

$$\text{AUC}_{\text{real}} \approx \sum_{i=1}^{n-1} \frac{C_{\text{real}}(t_i) + C_{\text{real}}(t_{i+1})}{2} (t_{i+1} - t_i)$$

$$\text{AUC}_{\text{sim}} \approx \sum_{i=1}^{n-1} \frac{C_{\text{sim}}(t_i) + C_{\text{sim}}(t_{i+1})}{2} (t_{i+1} - t_i)$$

Then we can define a **relative AUC error**:

$$\text{RE}_{\text{AUC}} = \left| \frac{\text{AUC}_{\text{sim}} - \text{AUC}_{\text{real}}}{\text{AUC}_{\text{real}}} \right| \times 100\%$$

If RE_{AUC} is small (for example, below 5%), we conclude that the simulation accurately reproduces the real drug exposure.

8. Case Study: Validating a Tumor Growth Simulation

8.1 Model Description

A simple tumor growth model:

$$\frac{dV}{dt} = rV\left(1 - \frac{V}{K}\right)$$

where:

- V is tumor volume,
- r is growth rate,
- K is carrying capacity.

8.2 Real Data

Measured tumor volume at days $\{1, 2, 3, 4\}$:

$$V_{\text{real}} = \{2.1, 3.0, 4.5, 6.2\}$$

8.3 Simulation Output

$$V_{\text{sim}} = \{2.0, 3.2, 4.8, 6.5\}$$

8.4 Pointwise Relative Error

For each time t_i, the **volumetric relative error** is:

$$\text{VRE}(t_i) = \frac{V_{\text{sim}}(t_i) - V_{\text{real}}(t_i)}{V_{\text{real}}(t_i)} \times 100\%$$

An overall tumor growth error can be defined as:

$$\text{Mean VRE} = \frac{1}{n}\sum_{i=1}^{n} |\text{VRE}(t_i)|$$

8.5 Correlation and R^2

We can also compute the correlation and R^2 between V_{real} and V_{sim}. Suppose:

$$r \approx 0.998, \qquad R^2 \approx 0.996$$

Very high values of r and R^2 indicate strong agreement and good validation.

9. Suggested Validation Workflow

1. Define validation criteria (acceptable error, e.g., RMSE, MAPE, R^2).
2. Collect real data or expert estimates.
3. Run simulation with identical conditions.
4. Compare results using numerical metrics and statistical tests.
5. Perform sensitivity analysis to check stability.
6. Decide whether to accept, reject, or refine the model.

10. Practical MATLAB/Python Example (Simple)

Python Implementation

```
import numpy as np

real = np.array([10, 7.5, 5.2, 3.1])
sim  = np.array([9.4, 7.0, 5.9, 3.4])

# RMSE
rmse = np.sqrt(np.mean((real - sim)**2))

# Bias
bias = np.mean(sim - real)

print("RMSE =", rmse)
print("Bias =", bias)

Output:
RMSE = 0.5454356057317856
Bias = -0.02499999999999991
```

11. Additional Topics (Suggested for Students)

- Cross-validation approaches in simulation.
- Bootstrapping simulation outputs.
- Validation under uncertainty.
- Expert-based validation vs. data-driven validation.

12. Conclusion

Validation is a core requirement in the simulation modeling cycle. A model is only as useful as its predictive accuracy. Using statistical measures (RMSE, MAPE, R^2, bias), visual comparison, sensitivity analysis, and expert judgment, we can determine whether a simulation model represents reality adequately.

A validated model improves decision-making, enhances system understanding, and ensures safety and reliability especially in critical domains such as medicine.