Mathematical Modeling with MATLAB

Gerardo Hernández
Application Engineer

Agenda

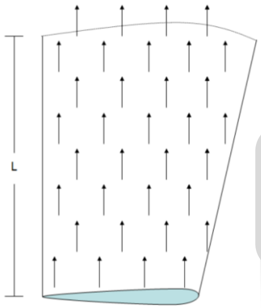
- Overview of mathematical modeling
- Mathematical modeling with MATLAB
  - Parametric modeling
  - Machine Learning (Black box)
- Summary

What is mathematical modeling?

- Use of mathematical language to describe a system or process

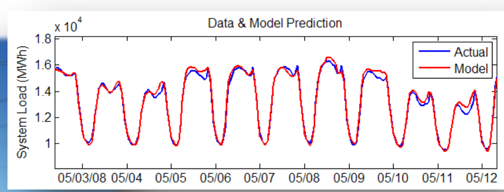
Input → **Mathematical model** → **Output**

- Some simple examples



$$q_l = \frac{2W_{to}n\sqrt{L^2 - x^2}}{L^2\pi}$$

Lift on aircraft wing



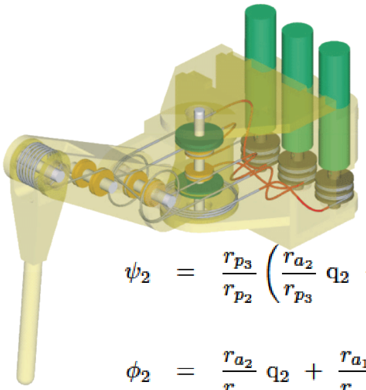
$$EL = f(T, t, DP, \ldots)$$

Electricity load

Why develop mathematical models?

- **Forecast system behavior**

  Predict and gain insight into system behavior for various “what-if” scenarios
  - Enables critical decisions
  - Reduces the need for testing



$$\psi_2 = \frac{r_{p_3}}{r_{p_2}}\left(\frac{r_{a_2}}{r_{p_3}}\,q_2 - \frac{r_{a_1}}{r_{p_1}}\,q_1\right)$$

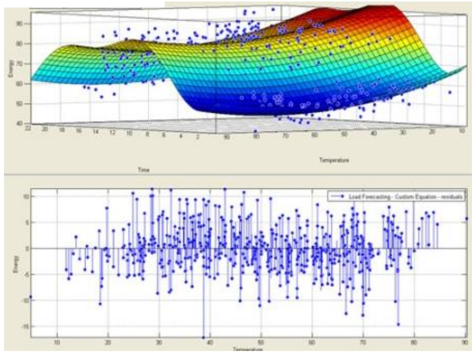
$$\phi_2 = \frac{r_{a_2}}{r_{p_2}}\,q_2 + \frac{r_{a_1}}{r_{p_1}}\left(\frac{r_{p_2} - r_{p_3}}{r_{p_2}}\right)q_1$$

- **Optimize system behavior**

  Identify parameters that optimize system performance

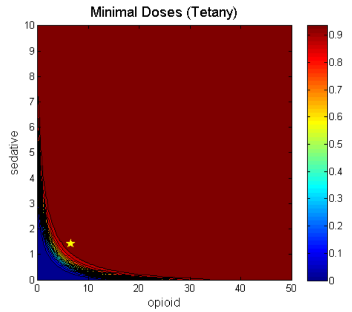
- **Design control systems**

  Develop model to represent plant during control system design

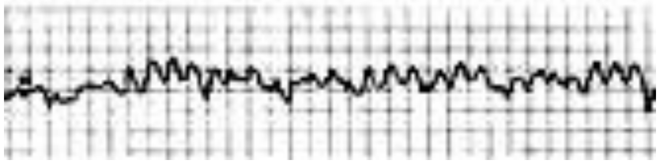


Demos

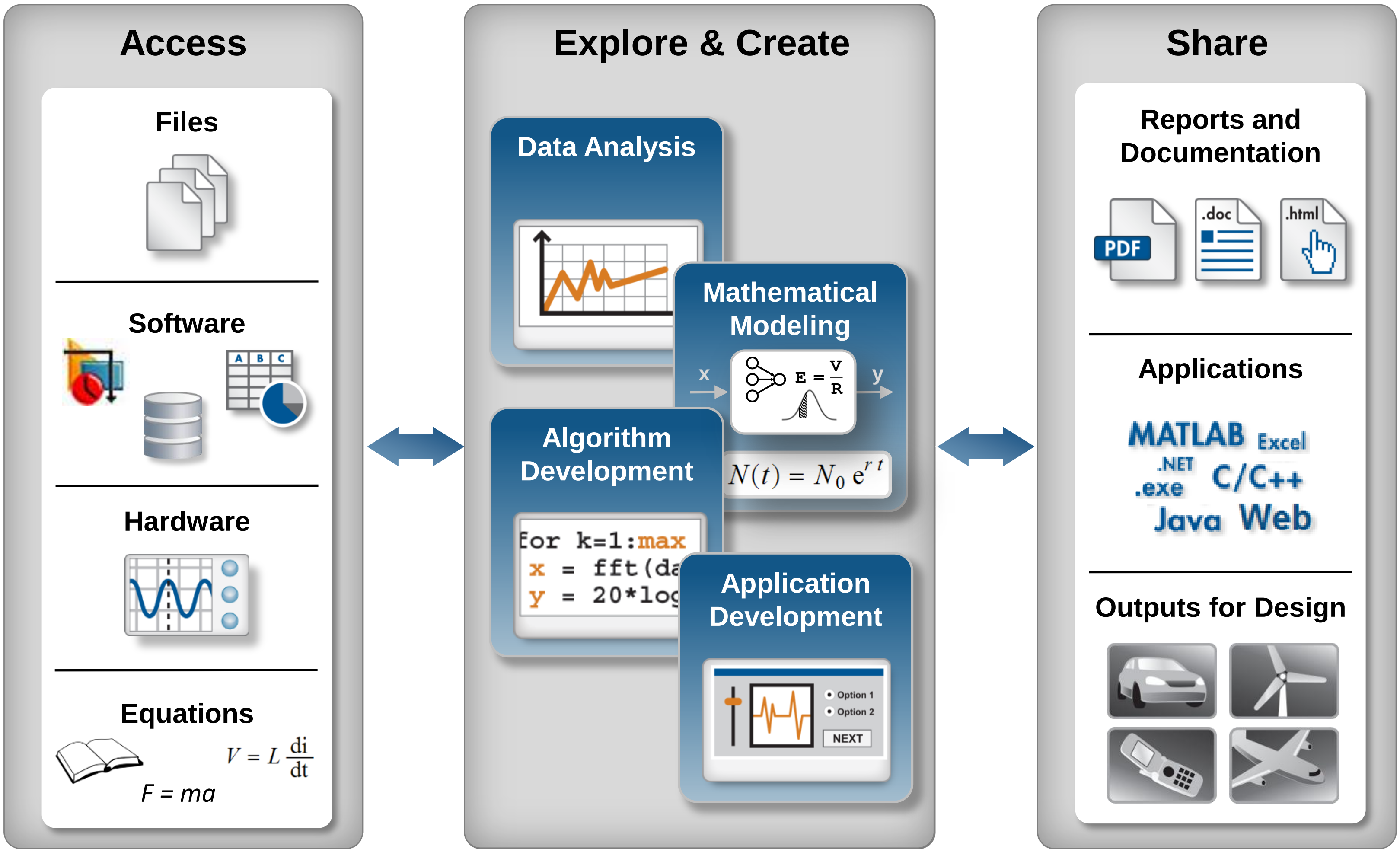
- Determining drug concentrations *(parametric)*
  - Surface fitting
  - Custom post-processing



- Detecting arrhythmia from ECG data *(black box modeling)*
  - Import and explore data
  - Partition data into test and training sets
  - Perform initial classification
  - Improve on classification using sequential feature selection
  - Document process in a report



Technical Computing with MATLAB Products

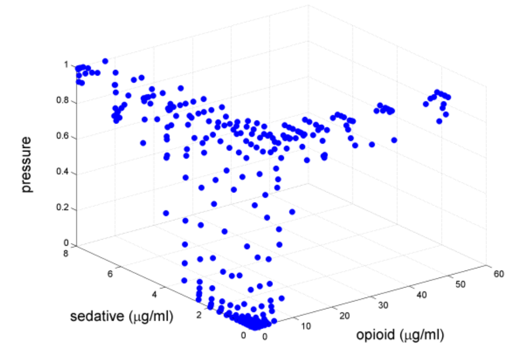


Agenda

- Overview of mathematical modeling
- Mathematical modeling with MATLAB
  - Parametric modeling
  - Machine Learning (Black box)
- Summary

Modeling Drug Interactions

- Determine minimal concentrations of opioid and sedative that produce effective anesthetic



$$R = \frac{\left(\frac{C_O}{IC50_O} + \frac{C_S}{IC50_S} + \alpha \frac{C_O}{IC50_O} \frac{C_S}{IC50_S} \right)^n}{1 + \left(\frac{C_O}{IC50_O} + \frac{C_S}{IC50_S} + \alpha \frac{C_O}{IC50_O} \frac{C_S}{IC50_S} \right)^n}$$

R : anesthetic response

C_O : opioid concentration (μg/ml)

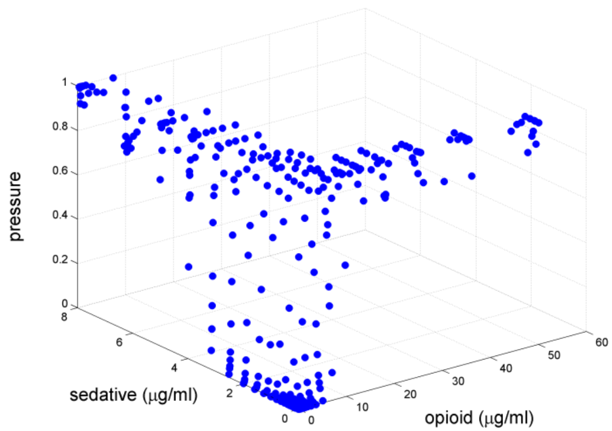
C_S : sedative concentration (μg/ml)

$IC50_O, IC50_S, \alpha, n$: model parameters

Modeling Drug Interactions

Products Used
- MATLAB
- Curve Fitting Toolbox

- Develop parametric model
  - Interactive surface fitting tool
  - Autogenerate code for fitting
- Identify optimal concentration
  - Use model to search parameter space
- Generate Report

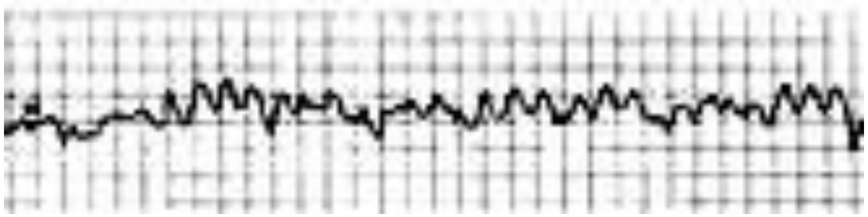


Agenda

- Overview of mathematical modeling
- Mathematical modeling with MATLAB
  - Parametric modeling
  - Machine Learning (Black box)
- Summary

Demo: Detecting arrhythmia from ECG data

- **Goal:**
  - Distinguish between the presence and absence of cardiac arrhythmia based on ECG data characteristics
- **Approach:**
  - Import and explore data
  - Partition data into test and training sets
  - Perform initial classification
  - Improve on classification using sequential feature selection
  - Document process in a report



Bache, K. & Lichman, M. (2013). UCI Machine Learning Repository [http://archive.ics.uci.edu/ml]. Irvine, CA: University of California, School of Information and Computer Science.

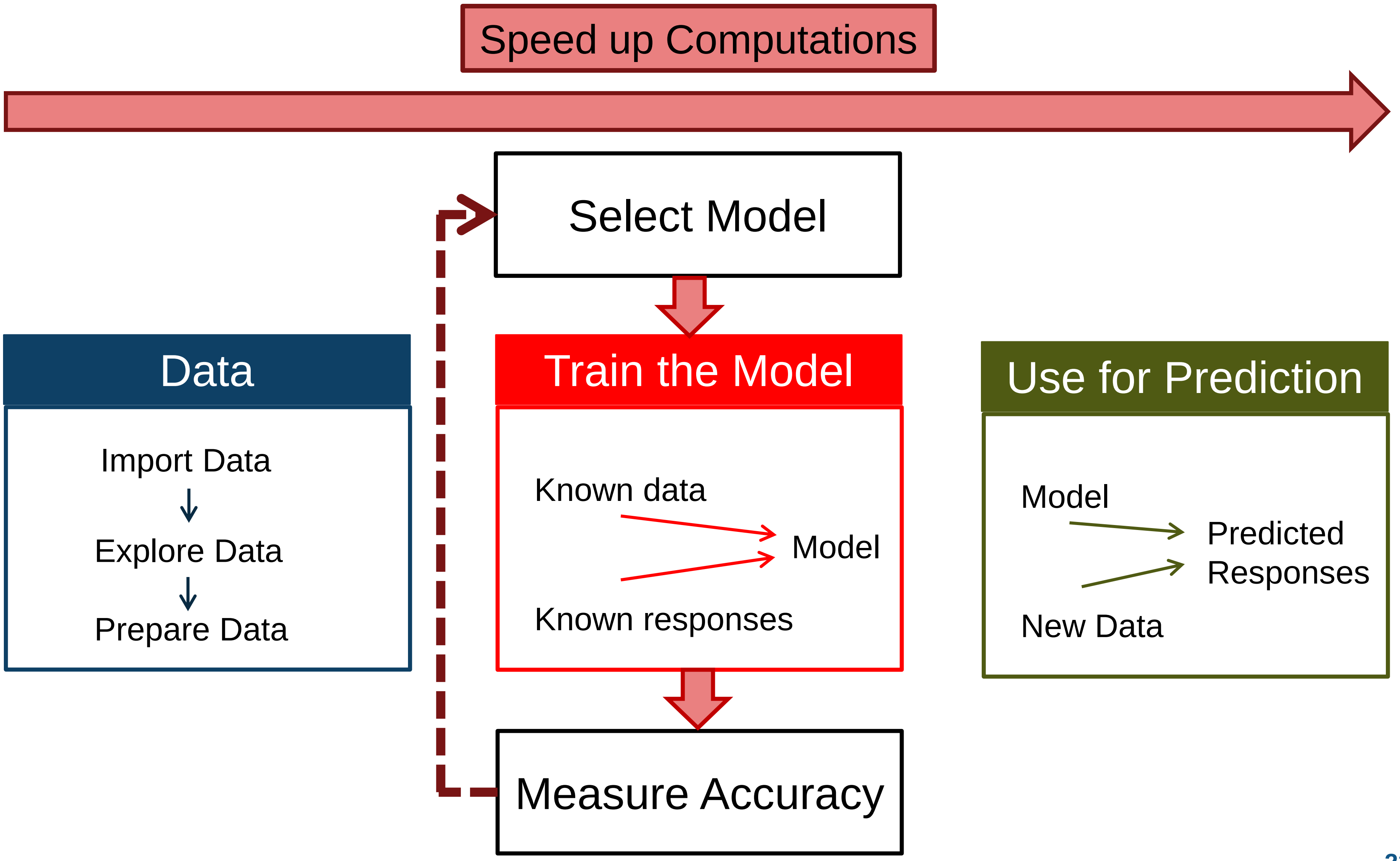
Challenges – Machine Learning

- Lots of data, with many variables (predictors)
- Data is too complex to know the governing equations
- Significant technical expertise required
- No “one size fits all” solution ➔ requires an iterative approach
  - Try multiple algorithms, see what works best
  - Time consuming

MATLAB Solution

- Strong environment for **interactive** exploration
- **Algorithms** and **Apps** to get started
  - Clustering, Classification, Regression
  - Neural network app, Curve fitting app
- Easy to evaluate, **iterate** and choose the best algorithm
- **Parallel computing**
- **Integrated** with data and deployment for Data Analytics workflows

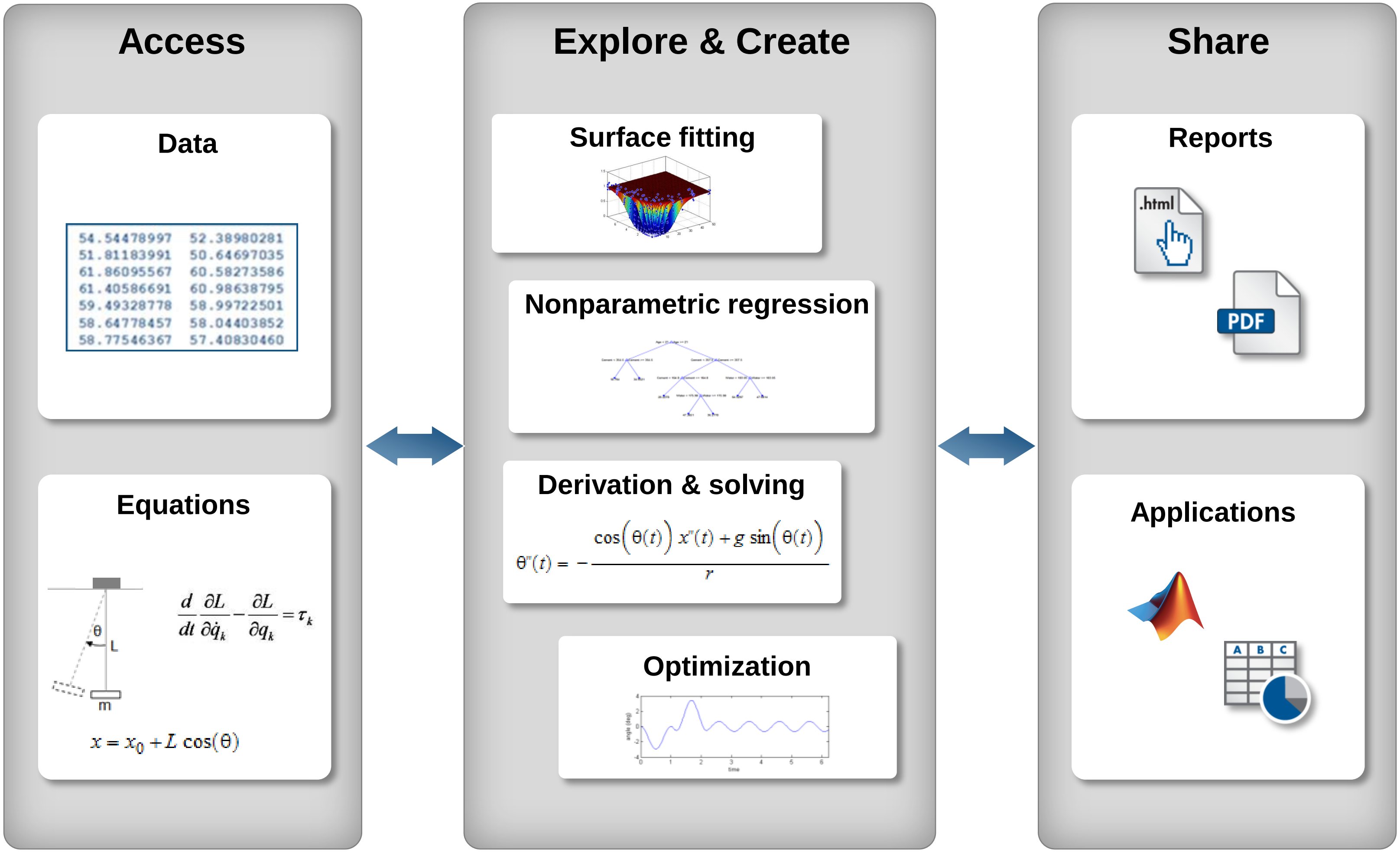
Supervised Learning - Workflow



Agenda

- Overview of mathematical modeling
- Mathematical modeling with MATLAB
  - Parametric modeling
  - Machine Learning (Black box)
- Summary

Mathematical Modeling with MATLAB

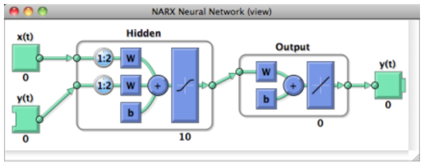


Building Mathematical Models in MATLAB

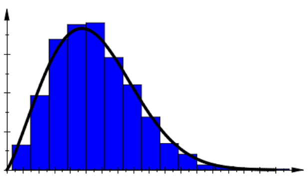
Toolboxes Extend Breadth of Modeling Tools

- Diverse modeling techniques
  - Deriving symbolic expressions
  - Fitting distributions
  - Linear and nonlinear regression
  - Machine learning (e.g. neural networks, decision trees)
  - Solving PDEs, ODEs

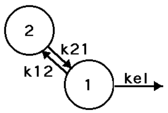
- Domain-specific
  - Financial (e.g. portfolio optimization, risk modeling)
  - Biological (e.g. pharmacokinetics, systems biology)



Neural network for time series data fitting



Weibull distribution for modeling wind speed



Pharmacokinetic model

Bond pricing model

Lund University Develops an Artificial Neural Network for Matching Heart Transplant Donors with Recipients

Challenge

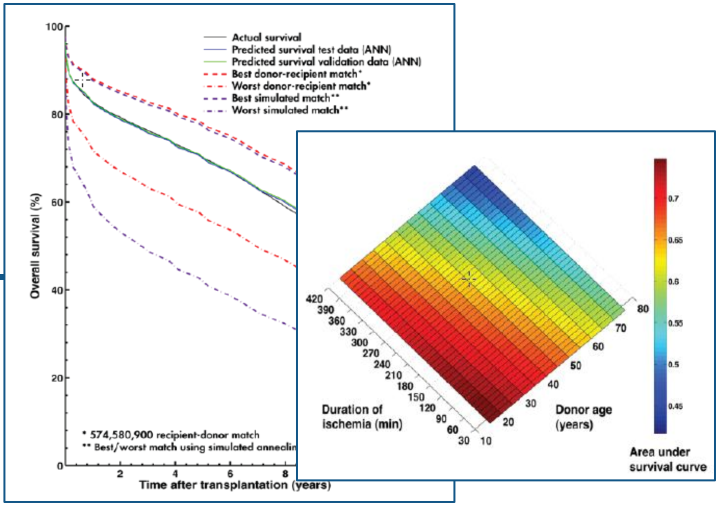
Improve long-term survival rates for heart transplant recipients by identifying optimal recipient and donor matches

Solution

Use MathWorks tools to develop a predictive artificial neural network model and simulate thousands of risk-profile combinations on a 56-processor computing cluster

Results

- Prospective five-year survival rate raised by up to 10%
- Network training time reduced by more than two-thirds
- Simulation time cut from weeks to days



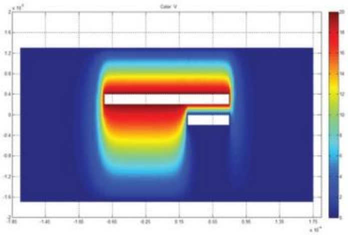
Plots showing actual and predicted survival, best and worst donor-recipient match, best and worst simulated match (left); and survival rate by duration of ischemia and donor age (right).

> **“I spend a lot of time in the clinic, and don’t have the time or the technical expertise to learn, configure, and maintain software. MATLAB makes it easy for physicians like me to get work done and produce meaningful results.”**
>
> **Dr. Johan Nilsson**
> **Skåne University Hospital**
> **Lund University**

[Link to user story]

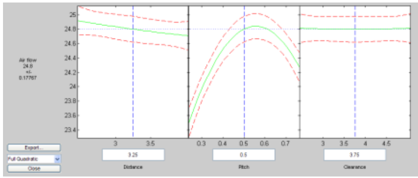
Learn More about Mathematical Modeling with MATLAB Products

- **MATLAB Digest**: *Accelerating Finite Element Analysis in MATLAB with Parallel Computing*

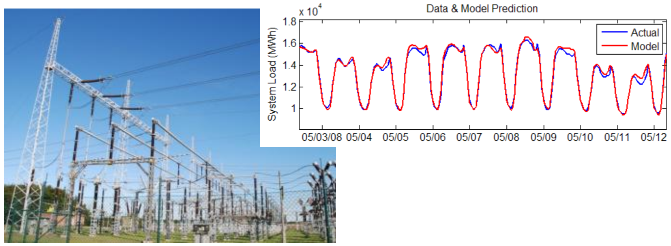


$$-\nabla \cdot (\varepsilon \nabla V) = \rho$$

- **MATLAB Digest**: *Improving an Engine Cooling Fan Using Design for Six Sigma Techniques*



- **Recorded webinar**: *Electricity Load and Price Forecasting with MATLAB*



- **Symbolic Math Toolbox Web demo**: *Modeling the Power Generated by a Wind Turbine*

$$\mathrm{Pe}_{\mathrm{ave}} = a \int_{u_c}^{u_r} f(u)\,\mathrm{d}u + b \int_{u_c}^{u_r} u^k f(u)\,\mathrm{d}u + \mathrm{Per} \int_{u_r}^{u_f} f(u)\,\mathrm{d}u$$

Support and Community

MathWorks | Book Program

MathWorks | Connections Program

MATLAB CENTRAL

MathWorks | Consulting Services

MathWorks | Training Services