THE UNIVERSITY OF WINNIPEG | Professional, Applied and Continuing Education

INTRODUCTION TO MACHINE LEARNING

DIT 45100

THE UNIVERSITY OF WINNIPEG

Professional, Applied and Continuing Education

Module 1
Introduction

Agenda

- Fundamentals of machine learning
- Tools and frameworks

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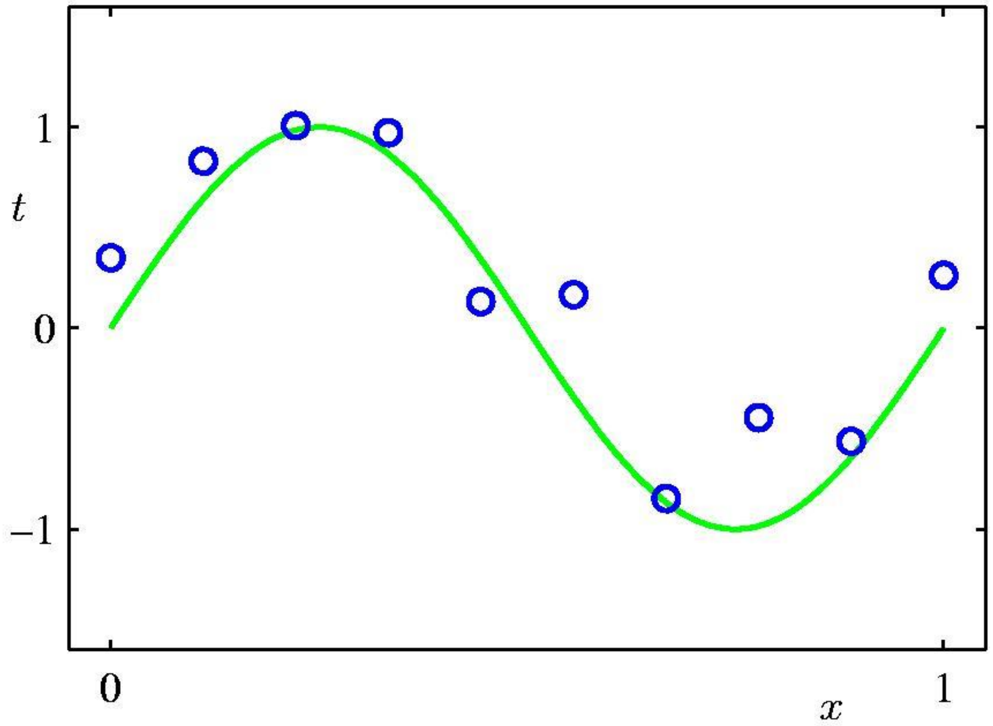
Fundamentals of Machine Learning

Fundamentals of ML

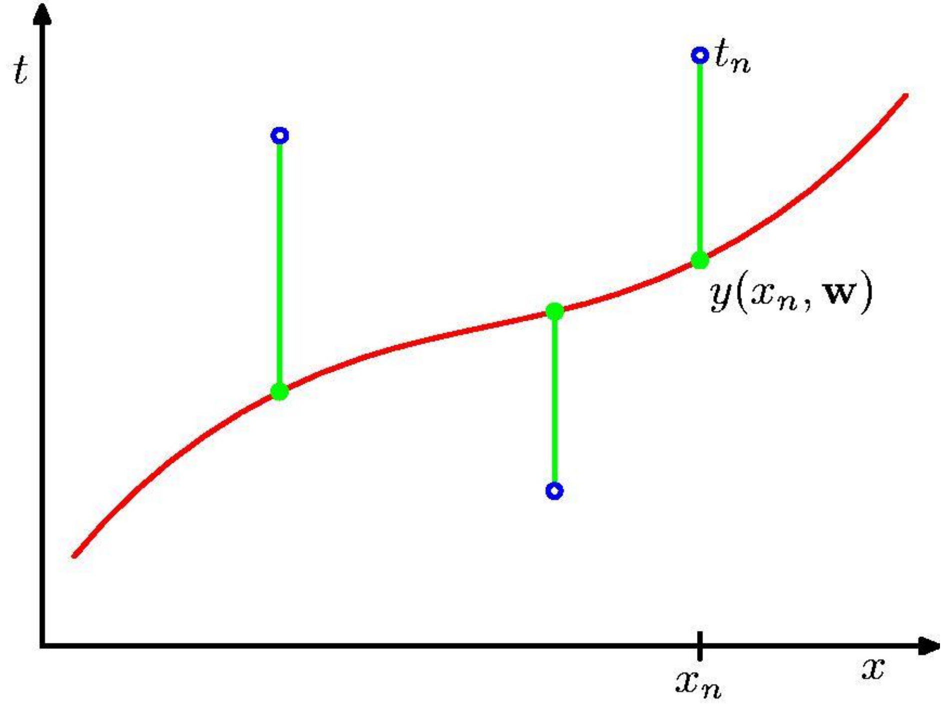
- Polynomial Curve Fitting
- Probability Theory
- Decision Theory
- Information Theory

Polynomial Curve Fitting



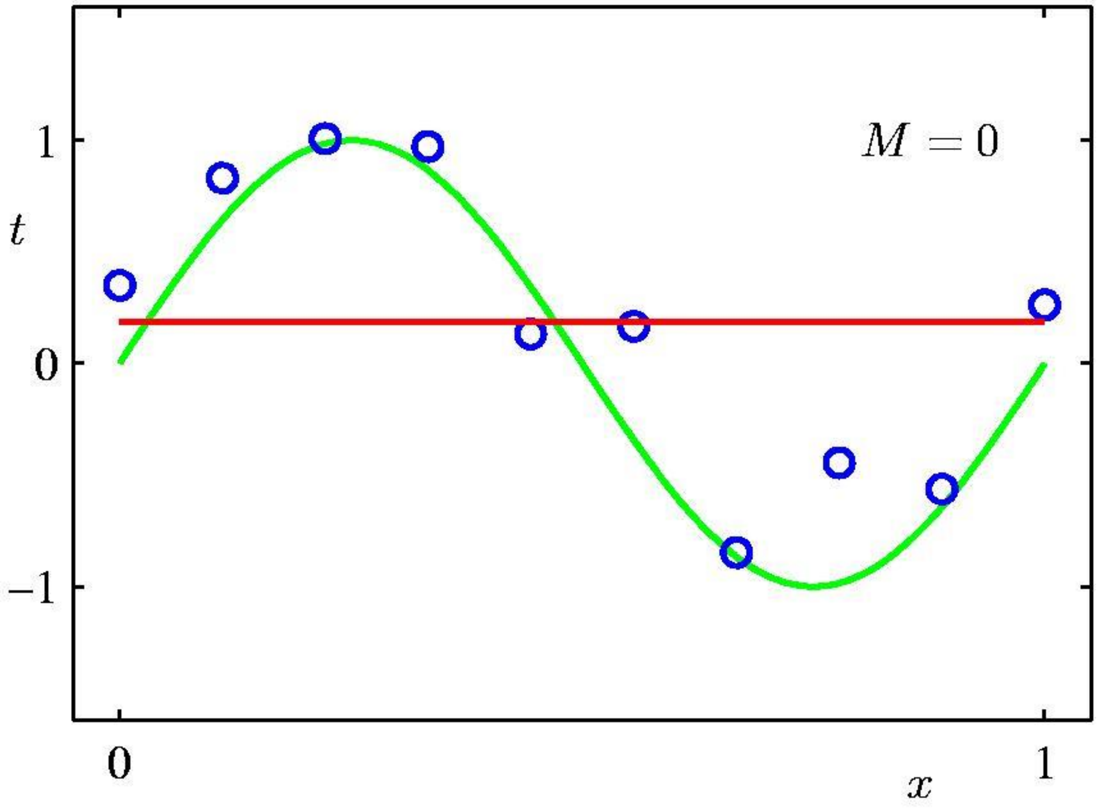
$$y(x, \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + \ldots + w_M x^M = \sum_{j=0}^{M} w_j x^j$$

Sum-of-Squares Error Function

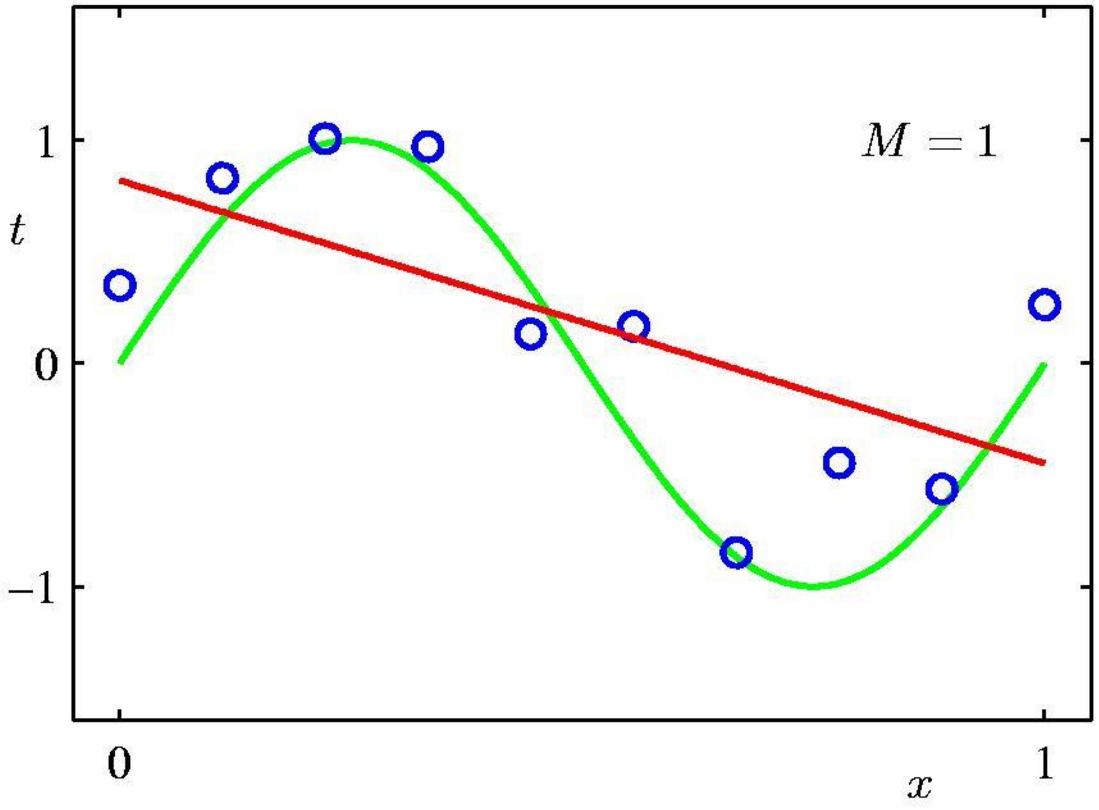


$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(x_n,\mathbf{w}) - t_n\}^2$$

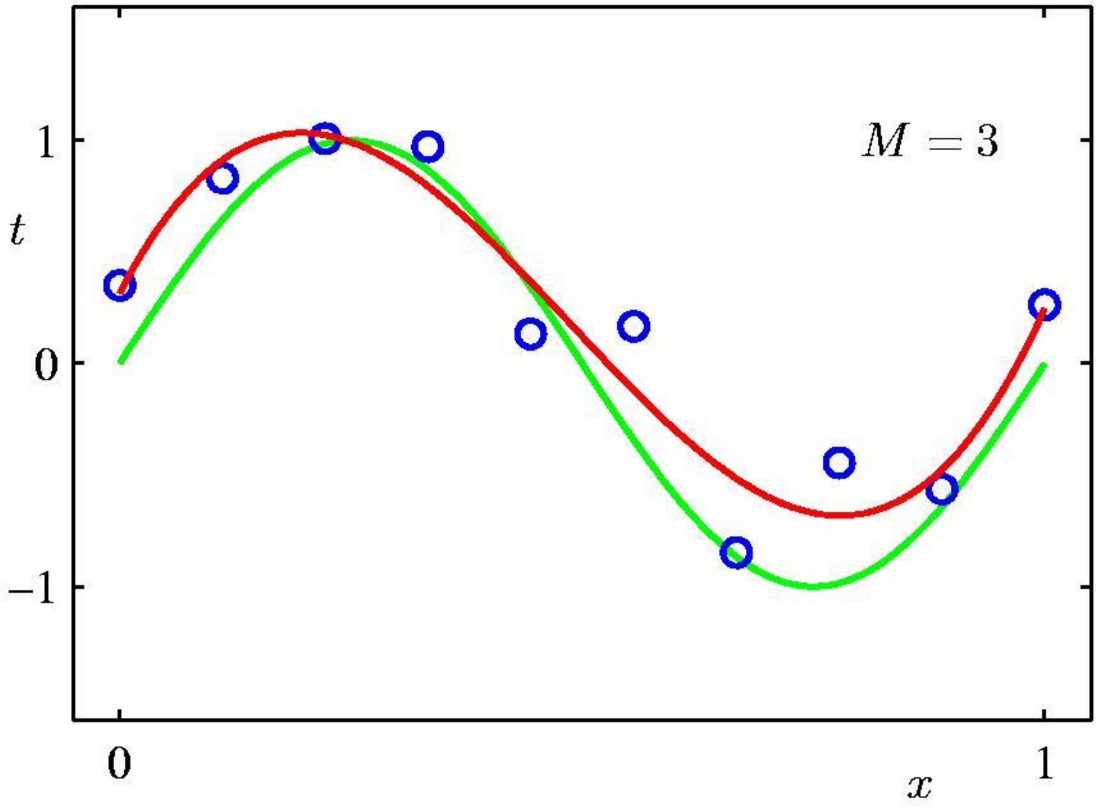
0th Order Polynomial



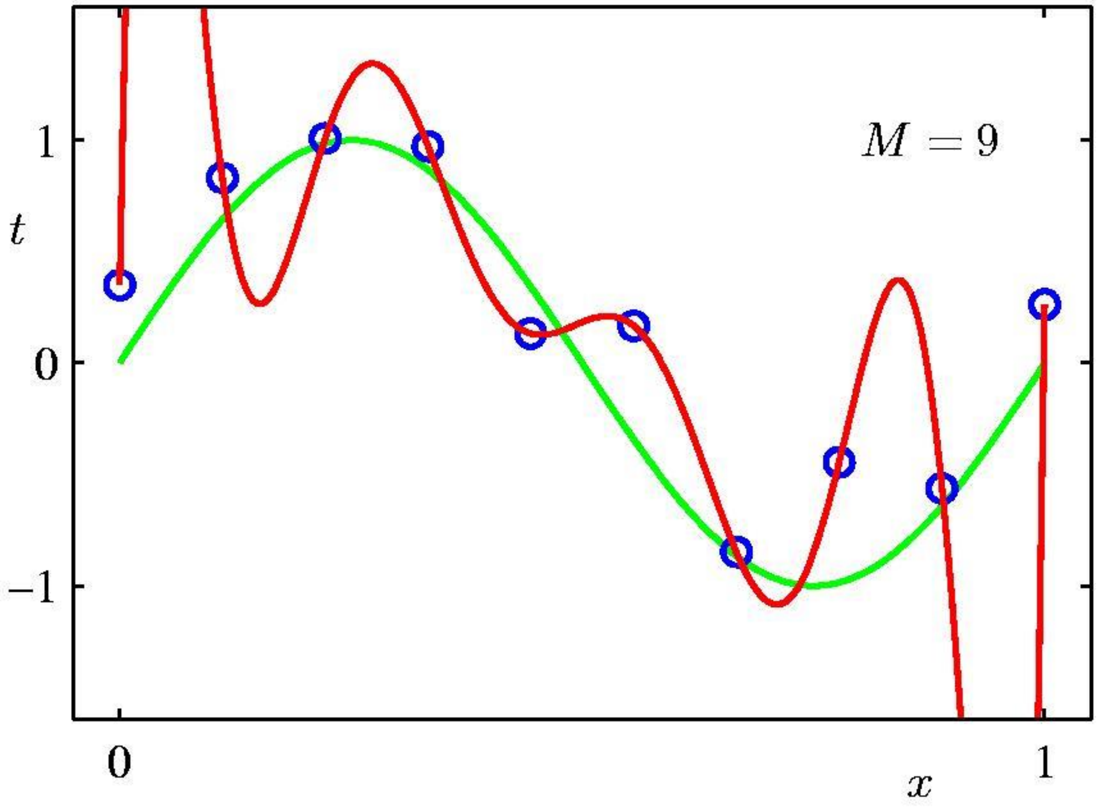
1st Order Polynomial



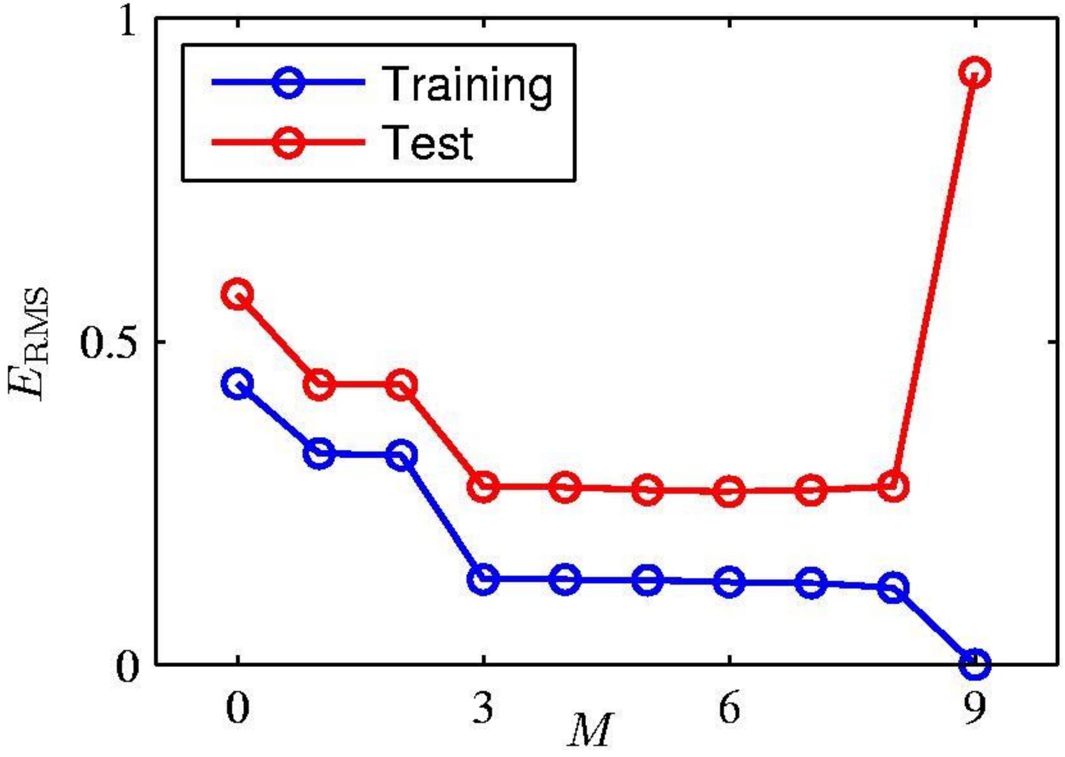
3rd Order Polynomial



9th Order Polynomial

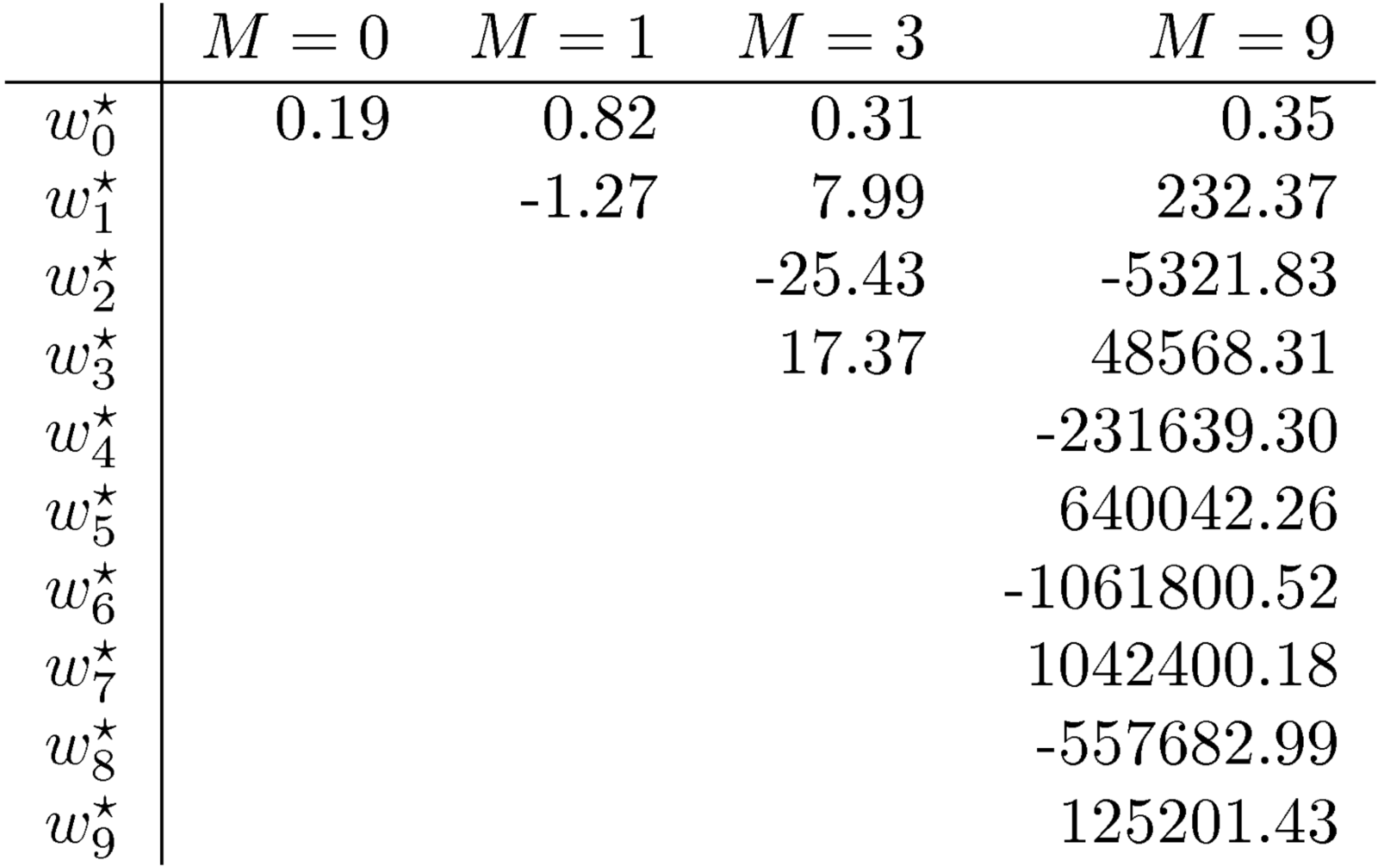


Over-fitting



Root-Mean-Square (RMS) Error: $E_{\mathrm{RMS}} = \sqrt{2E(\mathbf{w}^\star)/N}$

Polynomial Coefficients

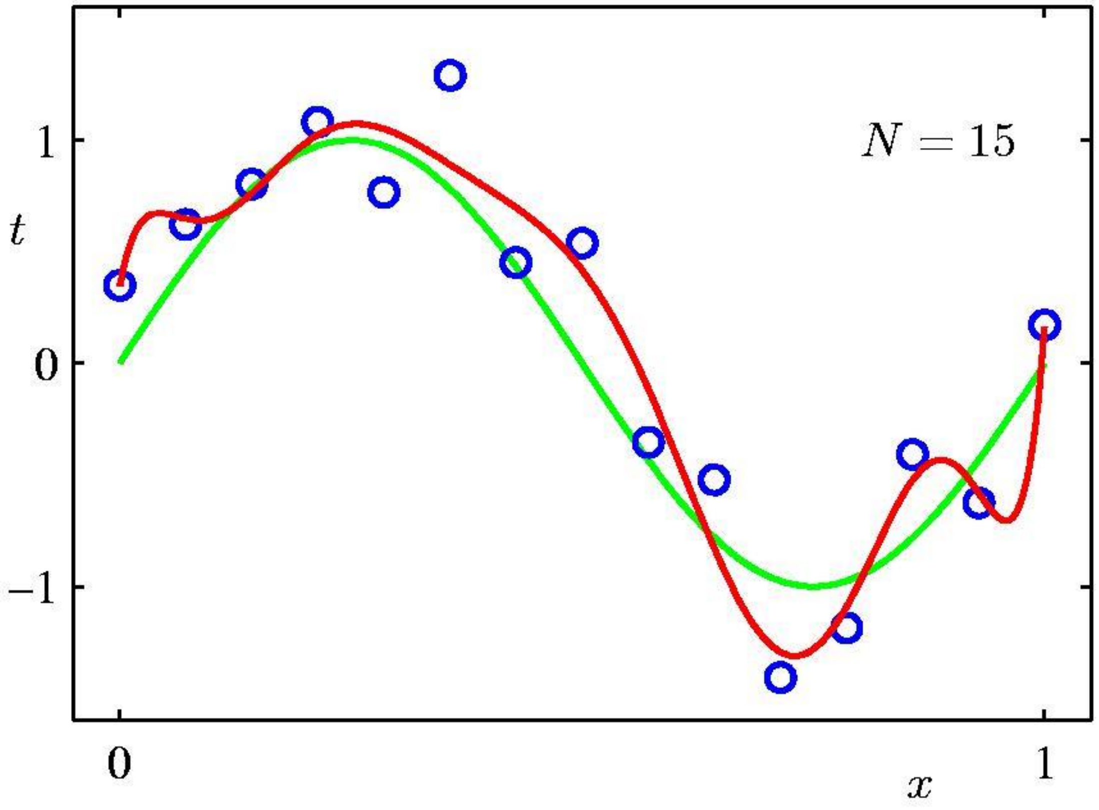


	$M = 0$	$M = 1$	$M = 3$	$M = 9$
$w_0^\star$	0.19	0.82	0.31	0.35
$w_1^\star$		-1.27	7.99	232.37
$w_2^\star$			-25.43	-5321.83
$w_3^\star$			17.37	48568.31
$w_4^\star$				-231639.30
$w_5^\star$				640042.26
$w_6^\star$				-1061800.52
$w_7^\star$				1042400.18
$w_8^\star$				-557682.99
$w_9^\star$				125201.43

Effect of Data Set Size

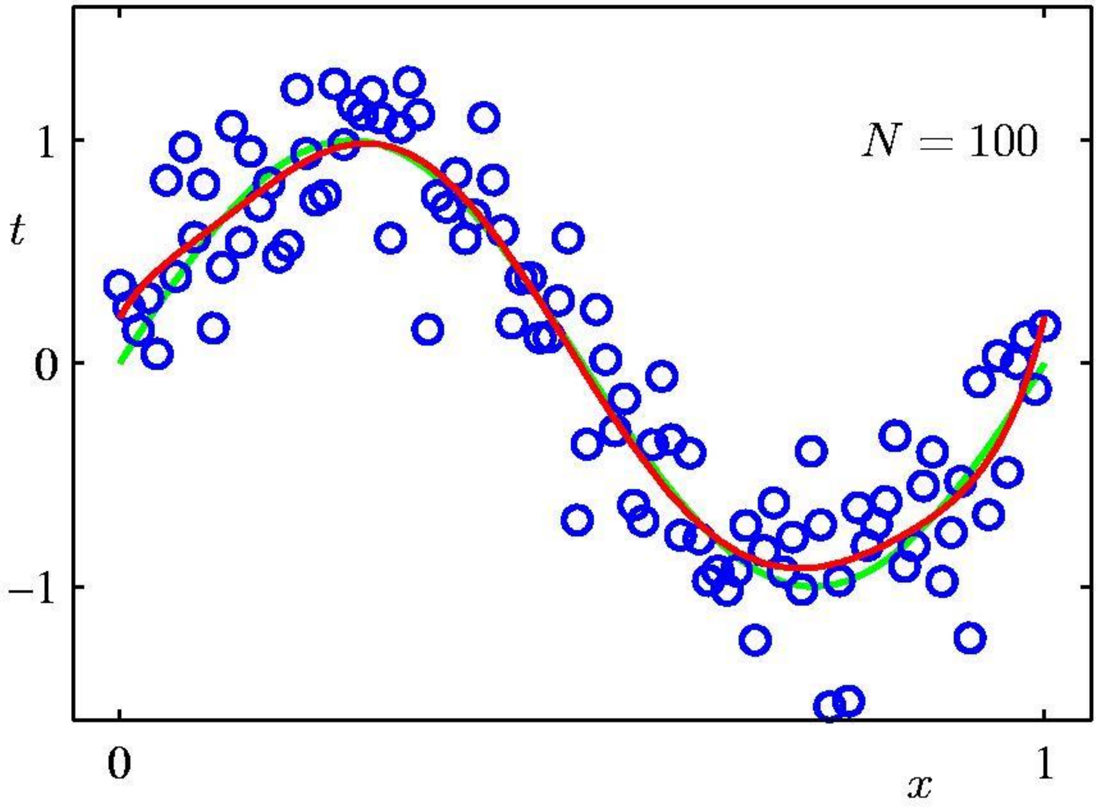
Data Set Size: $N = 15$

9th Order Polynomial



Data Set Size: $N = 100$

9th Order Polynomial



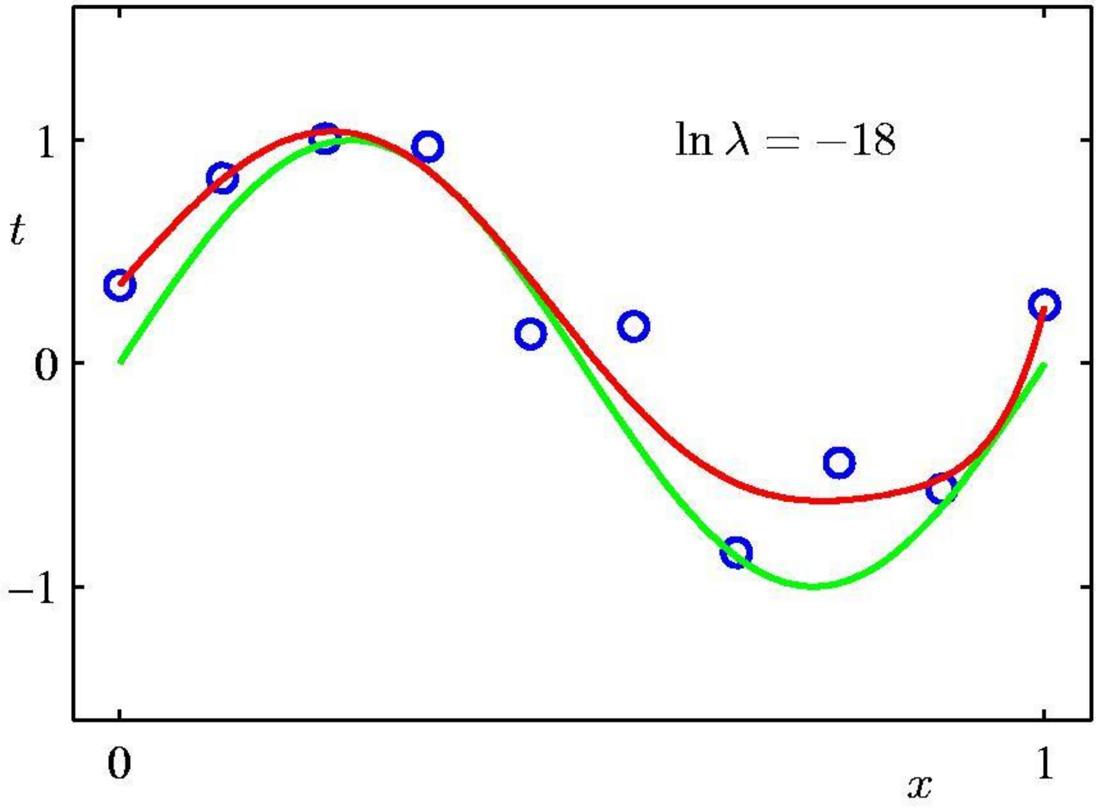
Regularization

Regularization

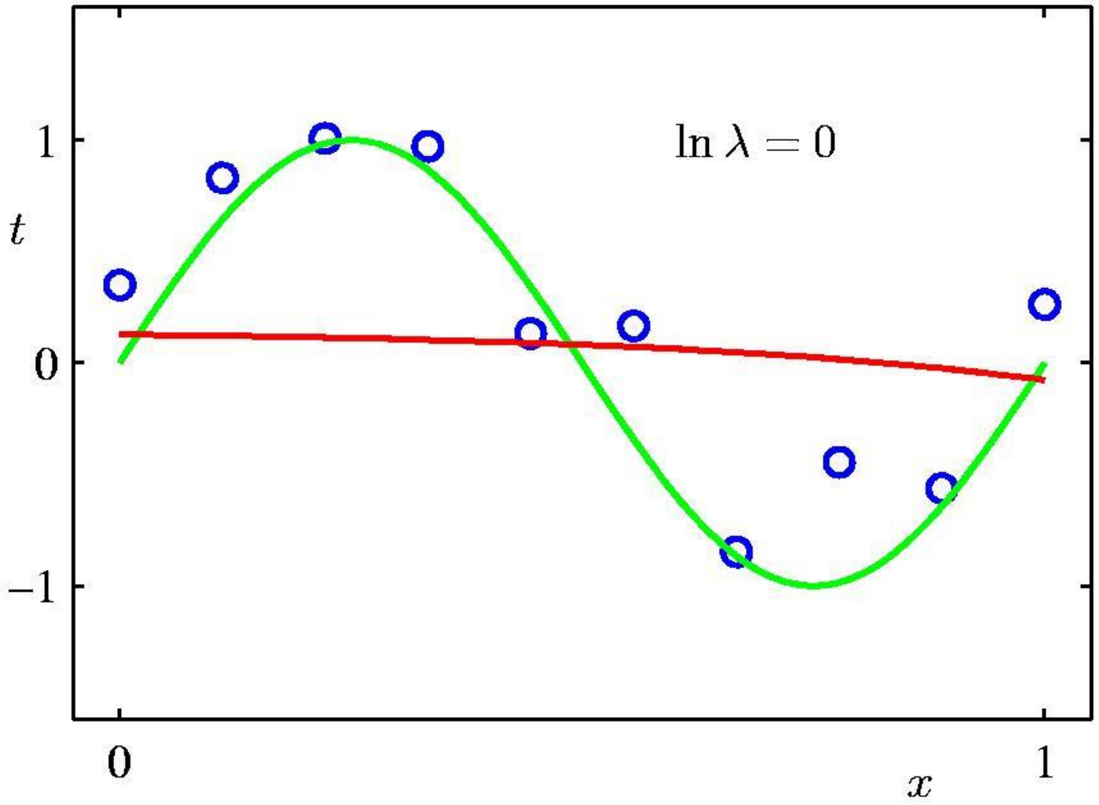
- Penalize large coefficient values

$$\widetilde{E}(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(x_n,\mathbf{w}) - t_n\}^2 + \frac{\lambda}{2}\|\mathbf{w}\|^2$$

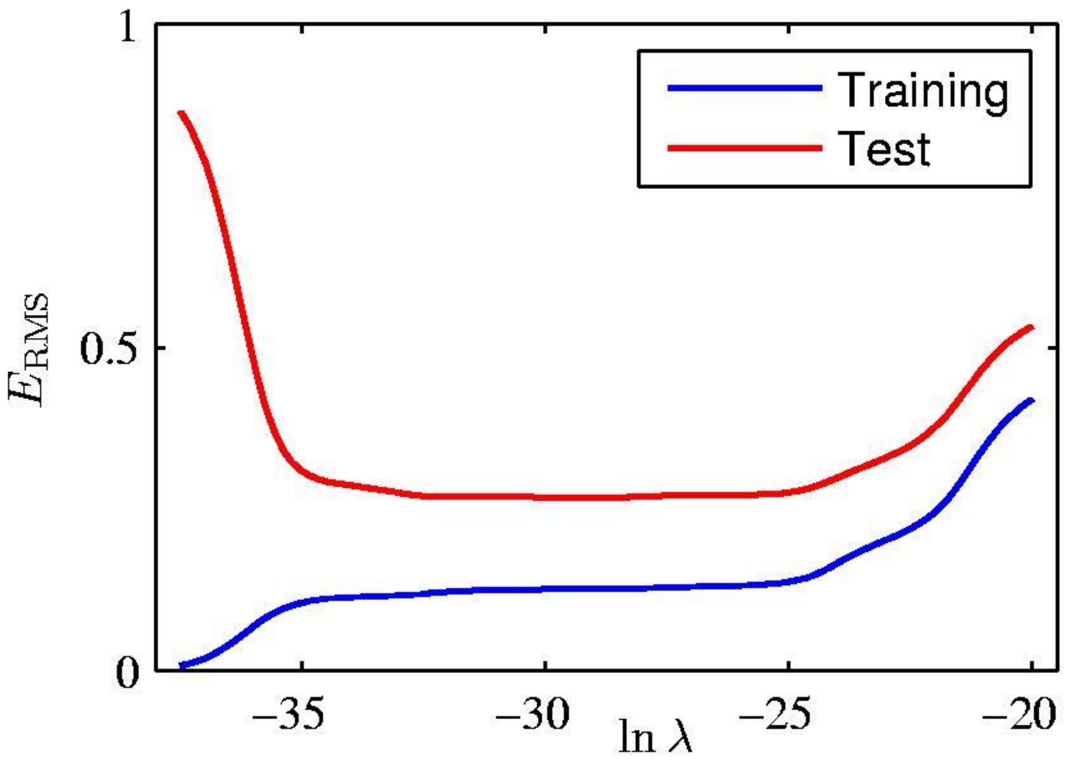
Regularization: $\ln\lambda = -18$



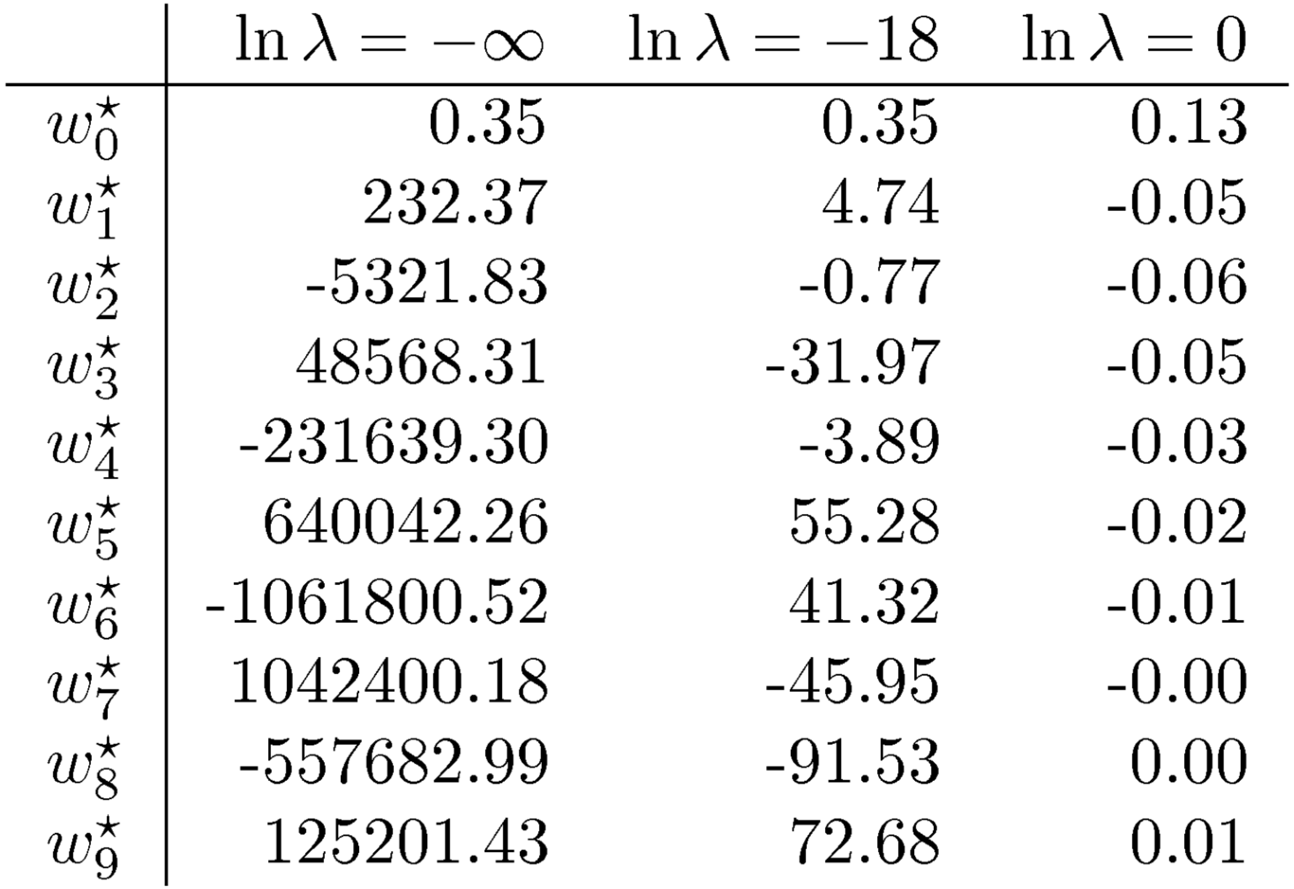
Regularization: $\ln \lambda = 0$



Regularization: E_{RMS} VS. ln λ



Polynomial Coefficients



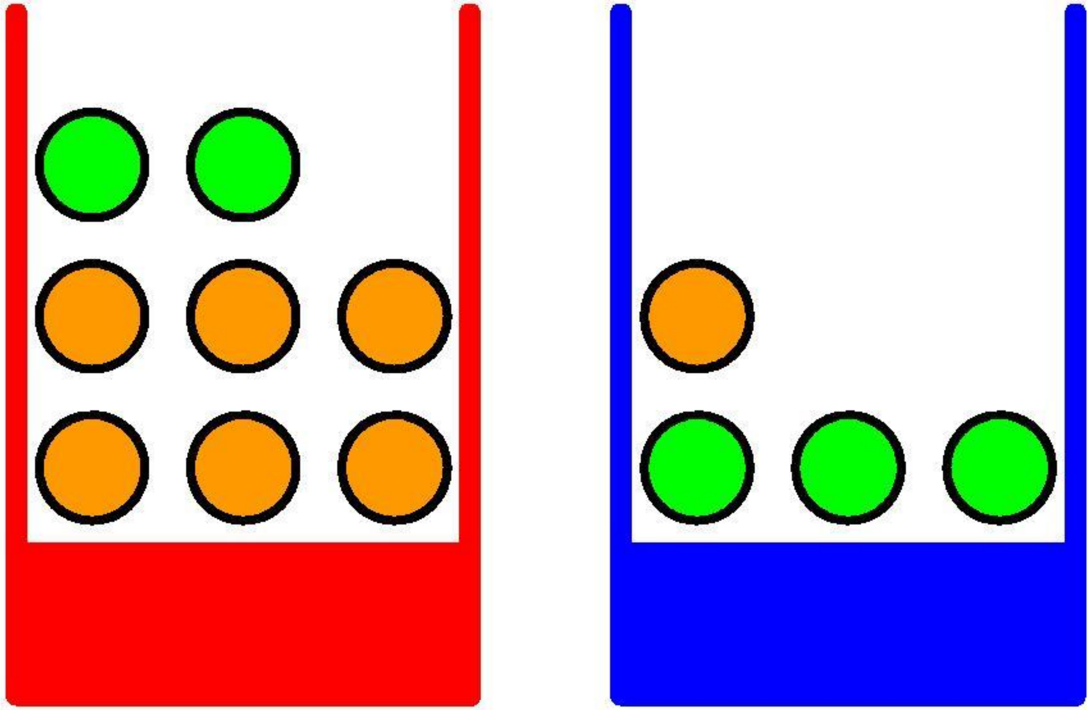
	$\ln\lambda = -\infty$	$\ln\lambda = -18$	$\ln\lambda = 0$
$w_0^\star$	0.35	0.35	0.13
$w_1^\star$	232.37	4.74	-0.05
$w_2^\star$	-5321.83	-0.77	-0.06
$w_3^\star$	48568.31	-31.97	-0.05
$w_4^\star$	-231639.30	-3.89	-0.03
$w_5^\star$	640042.26	55.28	-0.02
$w_6^\star$	-1061800.52	41.32	-0.01
$w_7^\star$	1042400.18	-45.95	-0.00
$w_8^\star$	-557682.99	-91.53	0.00
$w_9^\star$	125201.43	72.68	0.01

What Should I Know?

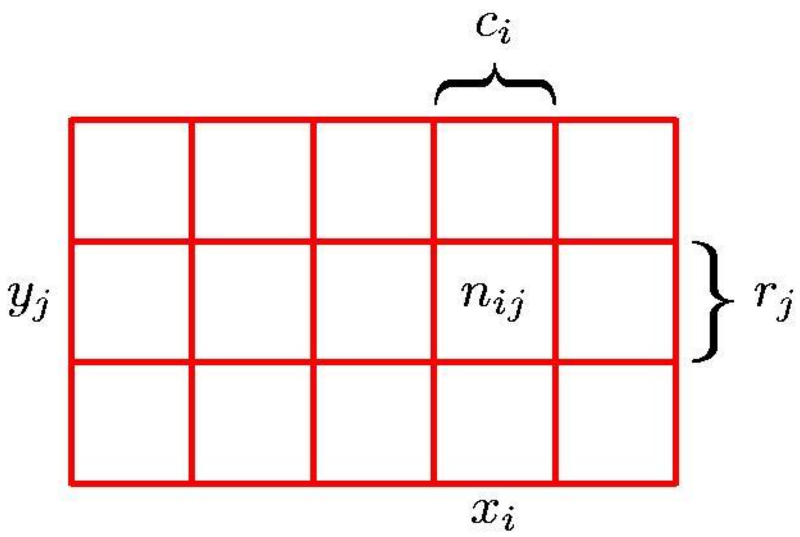
- Linear Algebra
- Derivatives
- Statistics
- Probability Theory
- Decision Theory
- Information Theory

Probability Theory

Apples and Oranges



Probability Theory



Marginal Probability

$$p(X = x_i) = \frac{c_i}{N}.$$

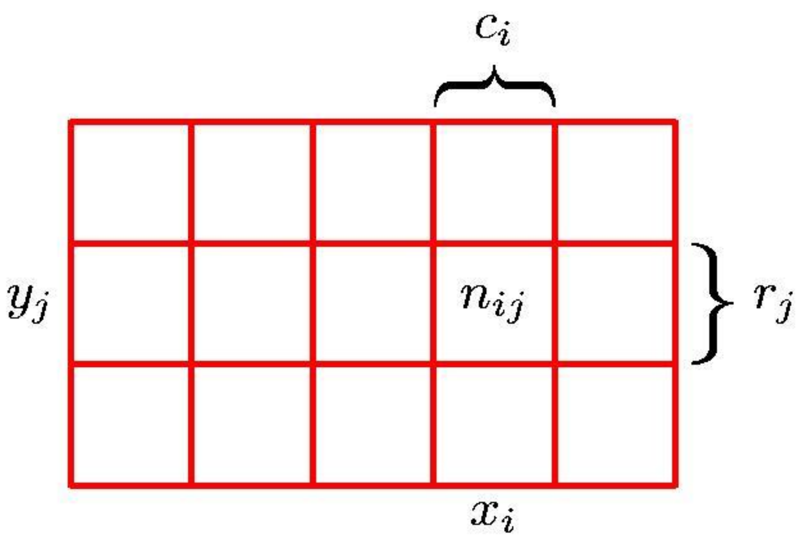
Joint Probability

$$p(X = x_i, Y = y_j) = \frac{n_{ij}}{N}$$

Conditional Probability

$$p(Y = y_j | X = x_i) = \frac{n_{ij}}{c_i}$$

Probability Theory



Sum Rule

$$p(X = x_i) = \frac{c_i}{N} = \frac{1}{N}\sum_{j=1}^{L} n_{ij}$$

$$= \sum_{j=1}^{L} p(X = x_i, Y = y_j)$$

Product Rule

$$\begin{aligned} p(X = x_i, Y = y_j) &= \frac{n_{ij}}{N} = \frac{n_{ij}}{c_i} \cdot \frac{c_i}{N} \\ &= p(Y = y_j | X = x_i)p(X = x_i) \end{aligned}$$

The Rules of Probability

Sum Rule	$p(X) = \sum_Y p(X, Y)$
Product Rule	$p(X, Y) = p(Y \mid X) p(X)$

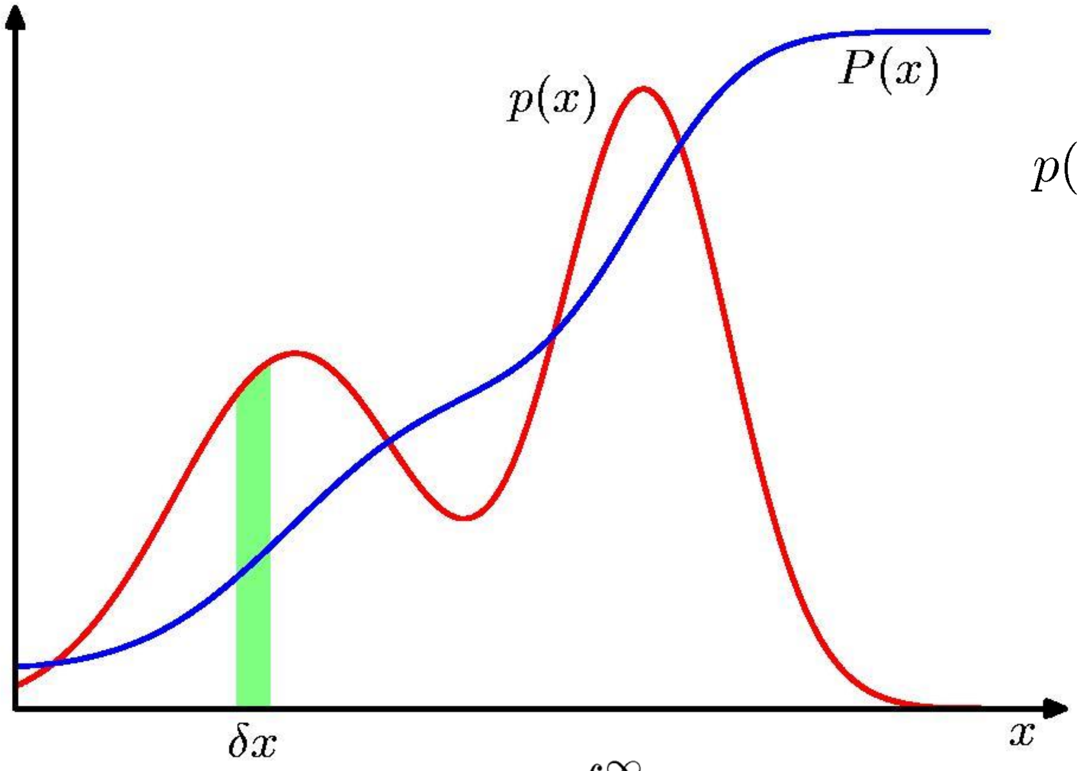
Bayes’ Theorem

$$p(Y|X) = \frac{p(X|Y)p(Y)}{p(X)}$$

$$p(X) = \sum_{Y} p(X|Y)p(Y)$$

posterior $\propto$ likelihood × prior

Probability Densities



$$p(x \in (a,b)) = \int_a^b p(x)\,\mathrm{d}x$$

$$P(z) = \int_{-\infty}^{z} p(x)\,\mathrm{d}x$$

$$p(x) \geqslant 0 \qquad \int_{-\infty}^{\infty} p(x)\,\mathrm{d}x = 1$$

Expectations

$$\mathbb{E}[f] = \sum_x p(x) f(x)$$

$$\mathbb{E}[f] = \int p(x) f(x) \, \mathrm{d}x$$

$$\mathbb{E}_x[f|y] = \sum_x p(x|y) f(x)$$

Conditional Expectation
(discrete)

$$\mathbb{E}[f] \simeq \frac{1}{N} \sum_{n=1}^{N} f(x_n)$$

Approximate Expectation
(discrete and continuous)

Variances and Covariances

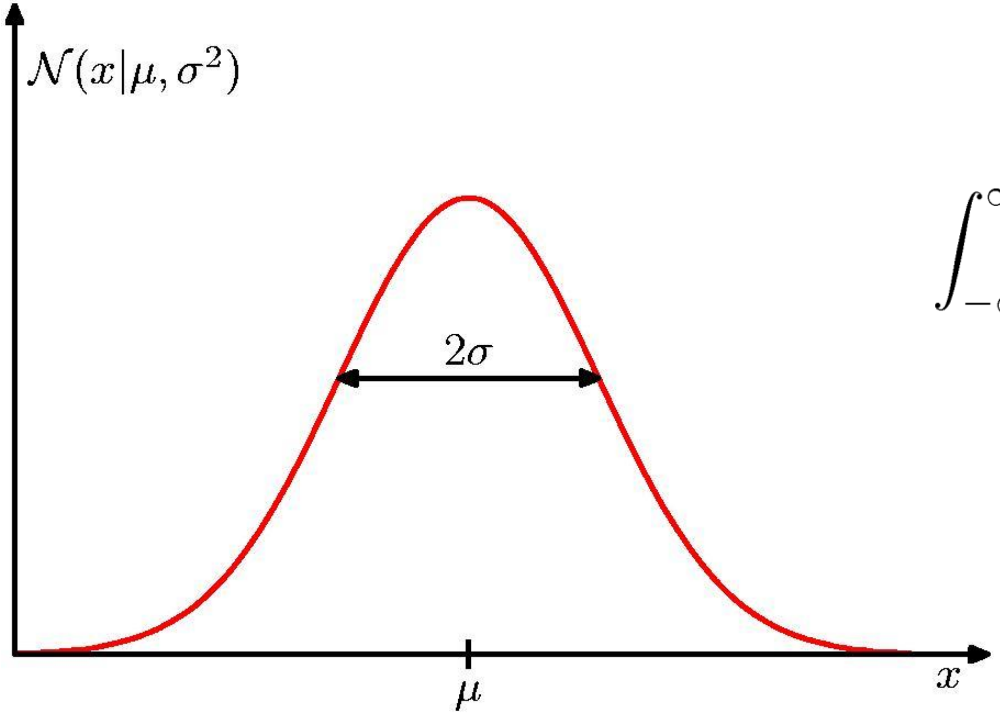
$$\mathrm{var}[f] = \mathbb{E}\left[\left(f(x) - \mathbb{E}[f(x)]\right)^2\right] = \mathbb{E}[f(x)^2] - \mathbb{E}[f(x)]^2$$

$$\begin{aligned}
\mathrm{cov}[x, y] &= \mathbb{E}_{x,y}\left[\{x - \mathbb{E}[x]\}\{y - \mathbb{E}[y]\}\right] \\
&= \mathbb{E}_{x,y}[xy] - \mathbb{E}[x]\mathbb{E}[y]
\end{aligned}$$

$$\begin{aligned}
\mathrm{cov}[\mathbf{x}, \mathbf{y}] &= \mathbb{E}_{\mathbf{x},\mathbf{y}}\left[\{\mathbf{x} - \mathbb{E}[\mathbf{x}]\}\{\mathbf{y}^{\mathrm{T}} - \mathbb{E}[\mathbf{y}^{\mathrm{T}}]\}\right] \\
&= \mathbb{E}_{\mathbf{x},\mathbf{y}}[\mathbf{x}\mathbf{y}^{\mathrm{T}}] - \mathbb{E}[\mathbf{x}]\mathbb{E}[\mathbf{y}^{\mathrm{T}}]
\end{aligned}$$

The Gaussian Distribution

$$\mathcal{N}\left(x|\mu,\sigma^2\right) = \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left\{-\frac{1}{2\sigma^2}(x-\mu)^2\right\}$$



$$\mathcal{N}(x|\mu,\sigma^2) > 0$$

$$\int_{-\infty}^{\infty} \mathcal{N}\left(x|\mu,\sigma^2\right)\,\mathrm{d}x = 1$$

Gaussian Mean and Variance

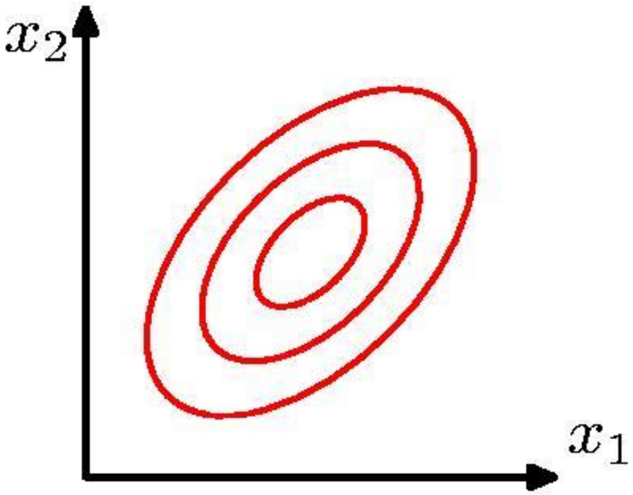
$$\mathbb{E}[x] = \int_{-\infty}^{\infty} \mathcal{N}\left(x|\mu, \sigma^2\right) x \,\mathrm{d}x = \mu$$

$$\mathbb{E}[x^2] = \int_{-\infty}^{\infty} \mathcal{N}\left(x|\mu, \sigma^2\right) x^2 \,\mathrm{d}x = \mu^2 + \sigma^2$$

$$\operatorname{var}[x] = \mathbb{E}[x^2] - \mathbb{E}[x]^2 = \sigma^2$$

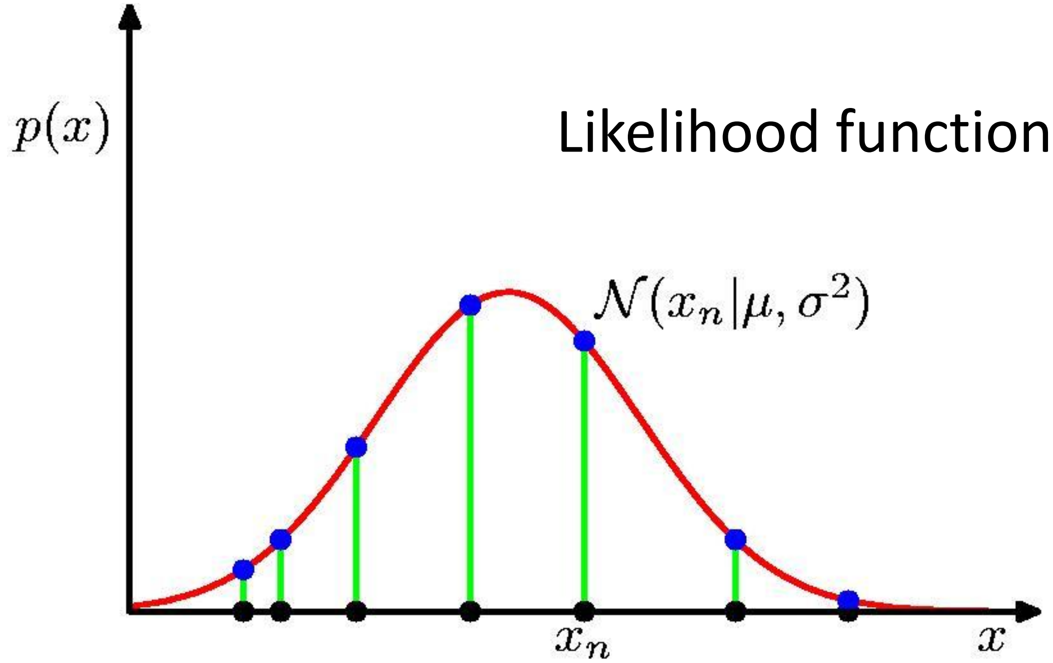
The Multivariate Gaussian

$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{D/2}}\frac{1}{|\boldsymbol{\Sigma}|^{1/2}}\exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\}$$



Gaussian Parameter Estimation

Likelihood function

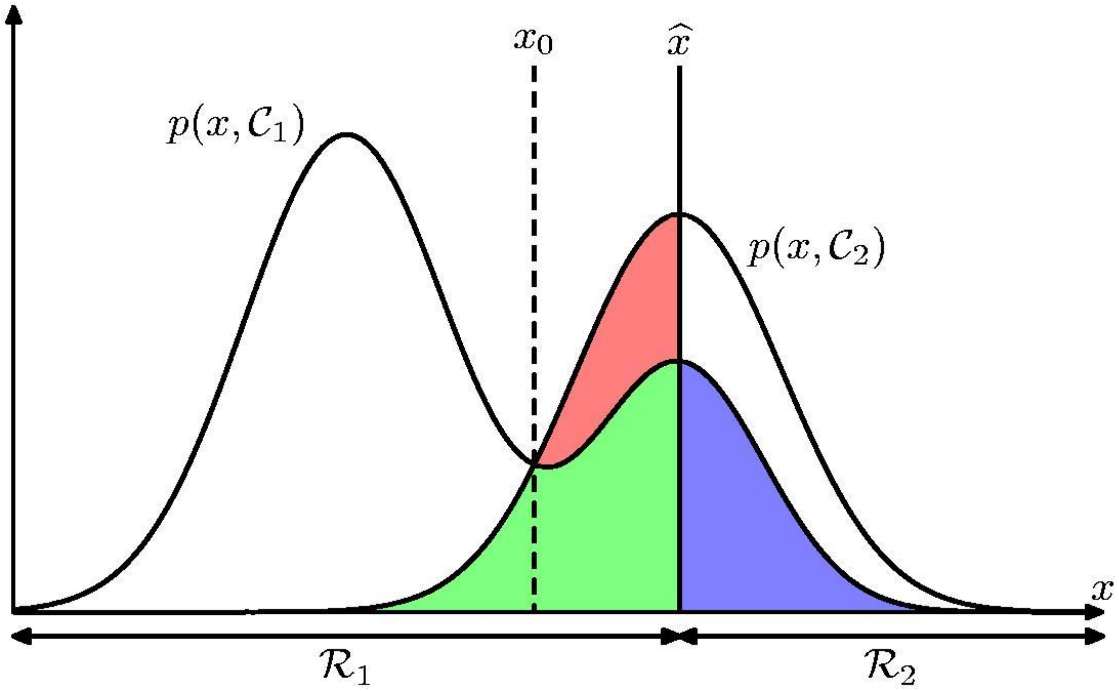


$$p(\mathbf{x}|\mu, \sigma^2) = \prod_{n=1}^{N} \mathcal{N}\left(x_n|\mu, \sigma^2\right)$$

Decision Theory

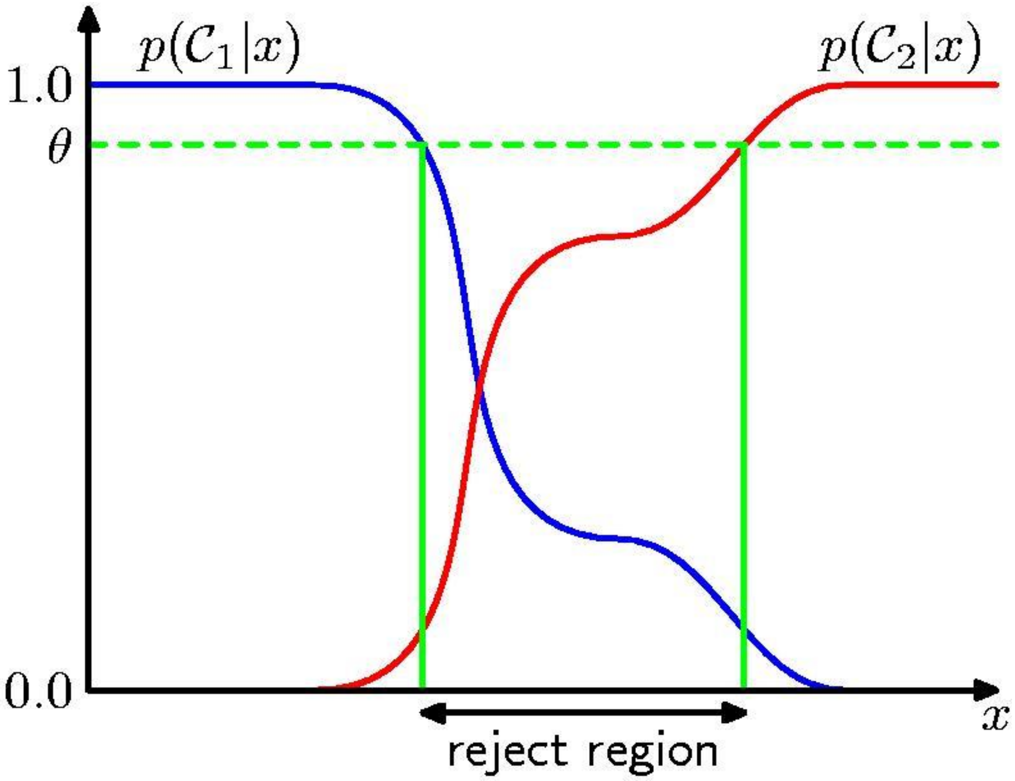
- Inference step
  - Determine either $p(t|\mathbf{x})$ or $p(\mathbf{x}, t)$
- Decision step
  - For given x, determine optimal t.

Minimum Misclassification Rate



$$\begin{aligned} p(\text{mistake}) &= p(\mathbf{x} \in \mathcal{R}_1, \mathcal{C}_2) + p(\mathbf{x} \in \mathcal{R}_2, \mathcal{C}_1) \\ &= \int_{\mathcal{R}_1} p(\mathbf{x}, \mathcal{C}_2)\,\mathrm{d}\mathbf{x} + \int_{\mathcal{R}_2} p(\mathbf{x}, \mathcal{C}_1)\,\mathrm{d}\mathbf{x}. \end{aligned}$$

Reject Option



Information Theory: Entropy

$$\mathrm{H}[x] = -\sum_{x} p(x) \log_2 p(x)$$

Important quantity in

- coding theory
- statistical physics
- machine learning

Entropy

- Coding theory: x discrete with 8 possible states; how many bits to transmit the state of x?

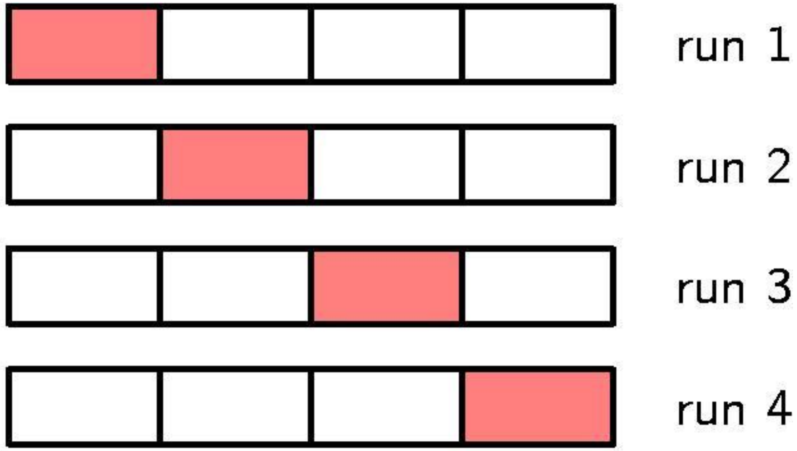
- All states equally likely

$$\mathrm{H}[x] = -8 \times \frac{1}{8} \log_2 \frac{1}{8} = 3 \text{ bits.}$$

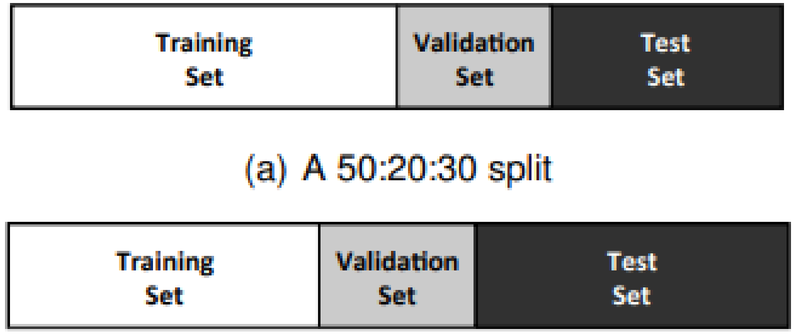
Supervised Learning Workflow

Model Selection

- Cross-Validation



Hold-out Sampling

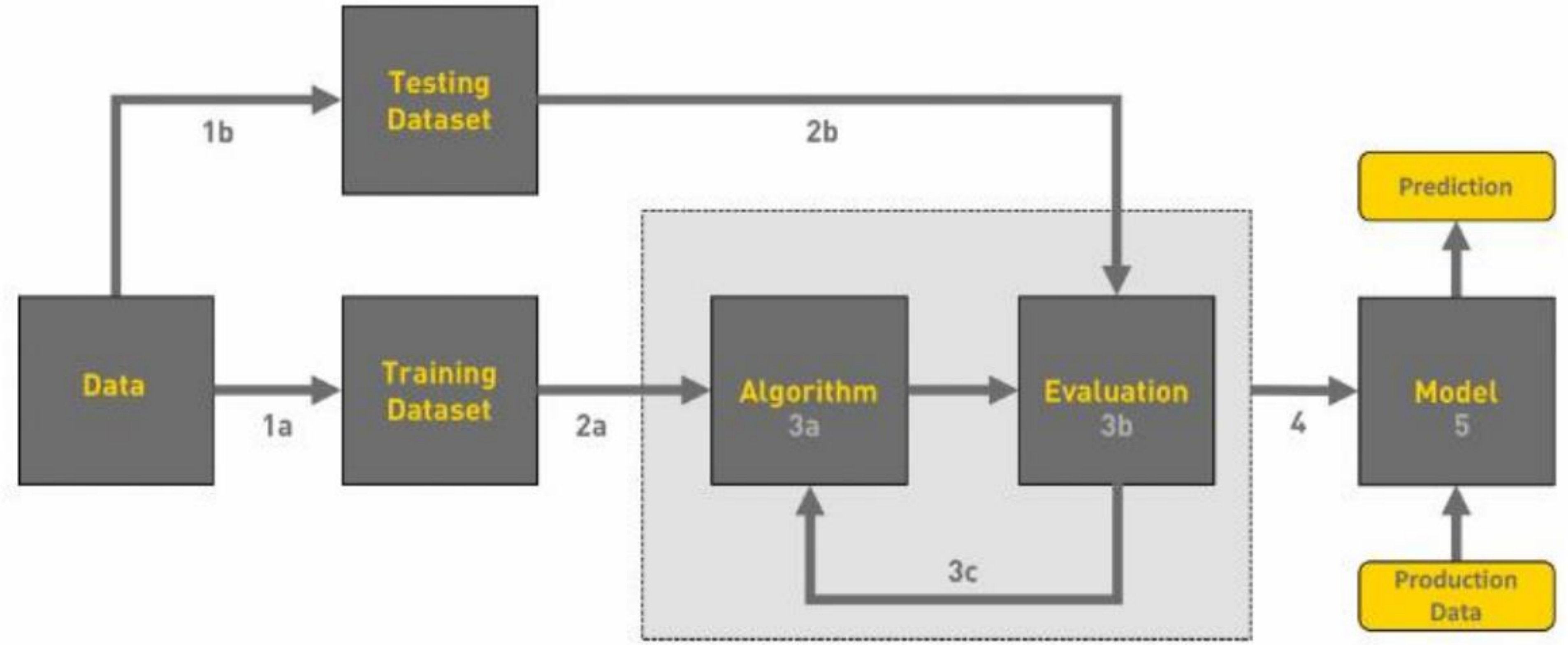


(a) A 50:20:30 split

(b) A 40:20:40 split

Figure: **Hold-out sampling** can divide the full data into training, validation, and test sets.

Workflow with Hold-out Sampling



Hold-out Sampling

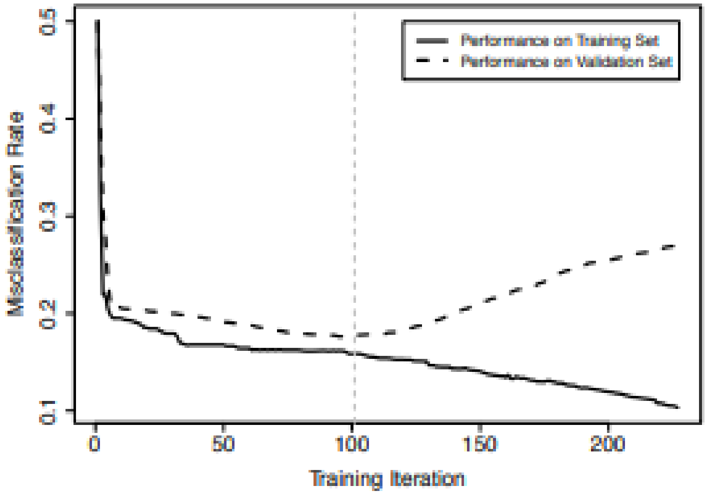
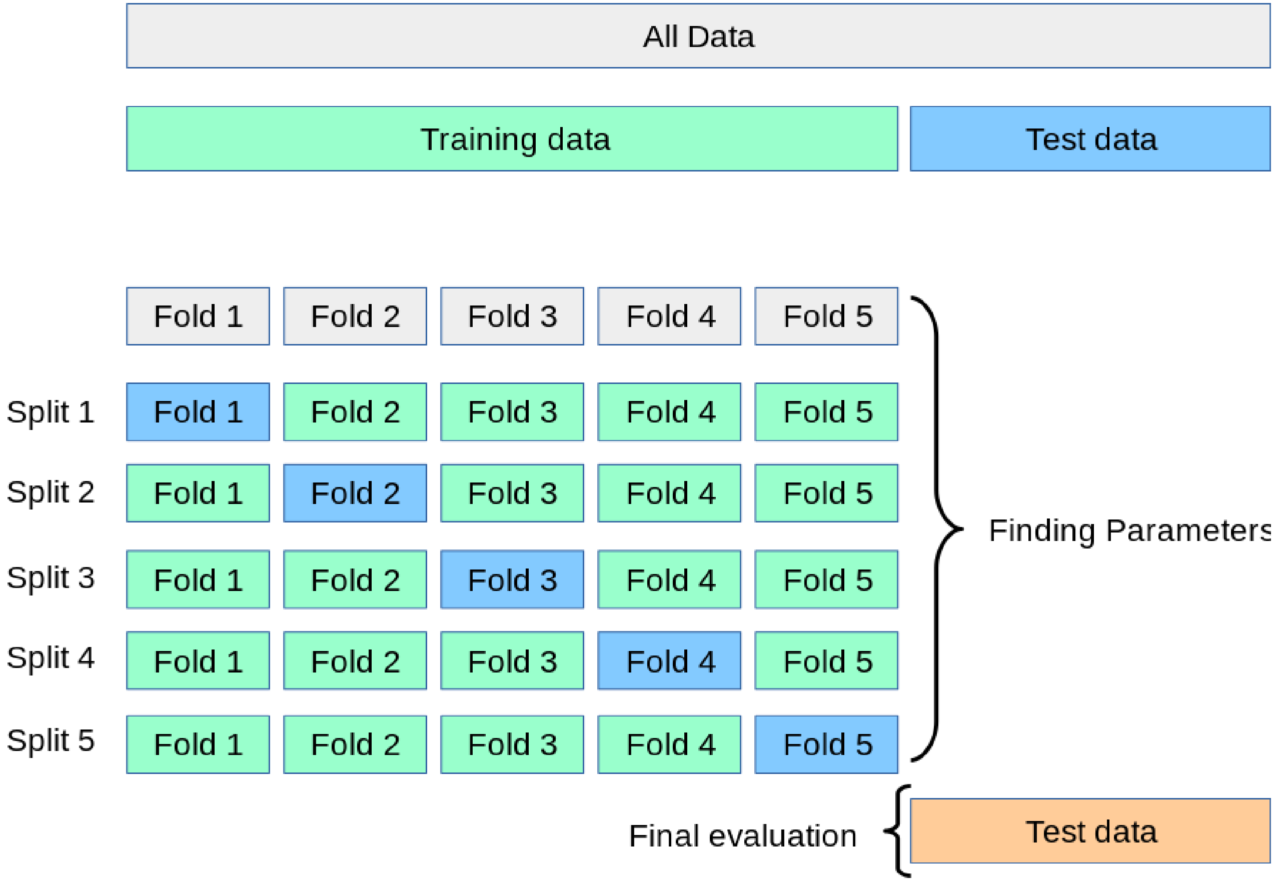


Figure: Using a validation set to avoid overfitting in iterative machine learning algorithms.

Cross Validation



All Data

Training data | Test data

Fold 1 | Fold 2 | Fold 3 | Fold 4 | Fold 5

Split 1 | Fold 1 | Fold 2 | Fold 3 | Fold 4 | Fold 5

Split 2 | Fold 1 | Fold 2 | Fold 3 | Fold 4 | Fold 5

Split 3 | Fold 1 | Fold 2 | Fold 3 | Fold 4 | Fold 5

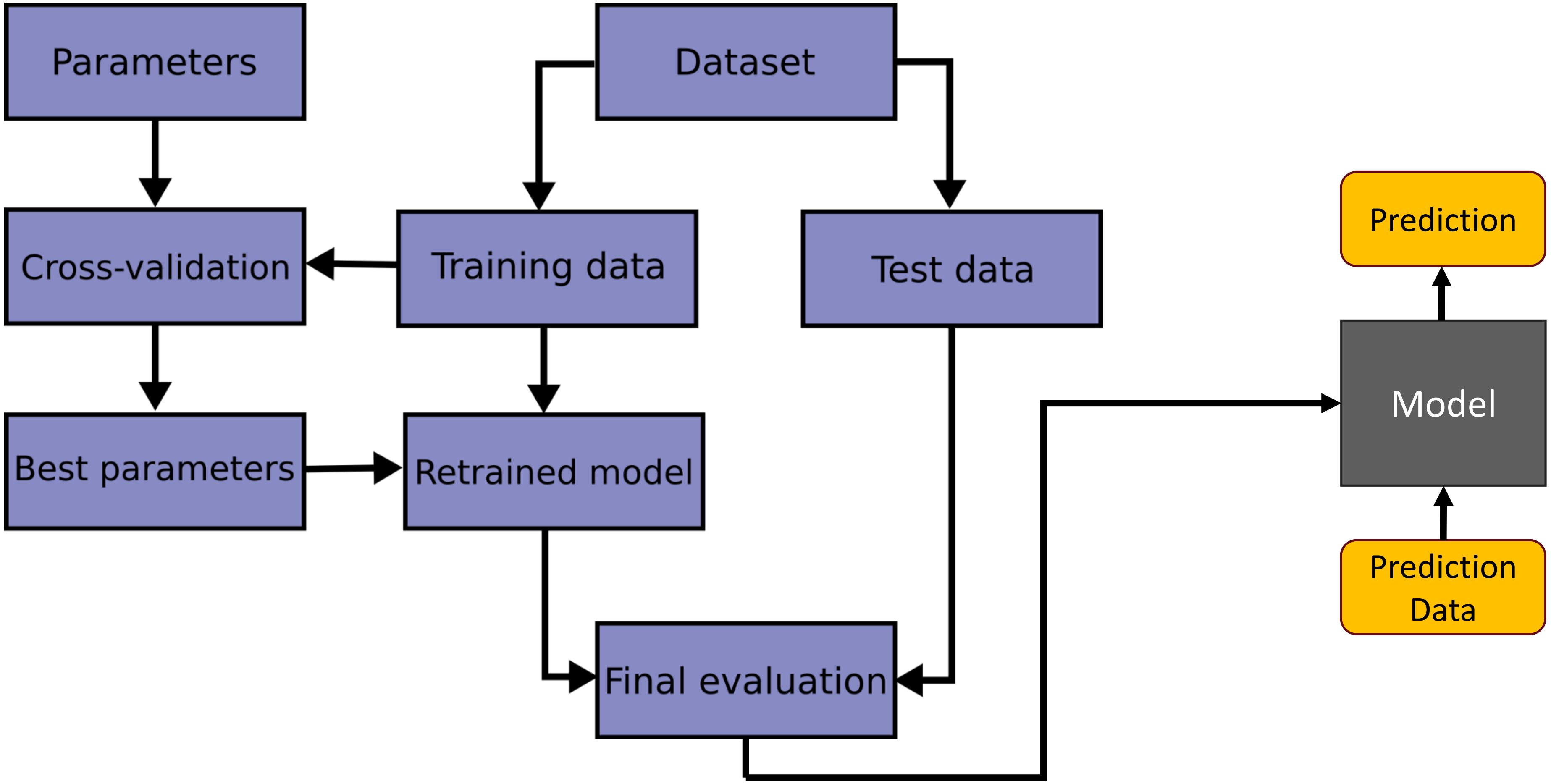
Split 4 | Fold 1 | Fold 2 | Fold 3 | Fold 4 | Fold 5

Split 5 | Fold 1 | Fold 2 | Fold 3 | Fold 4 | Fold 5

Finding Parameters

Final evaluation | Test data

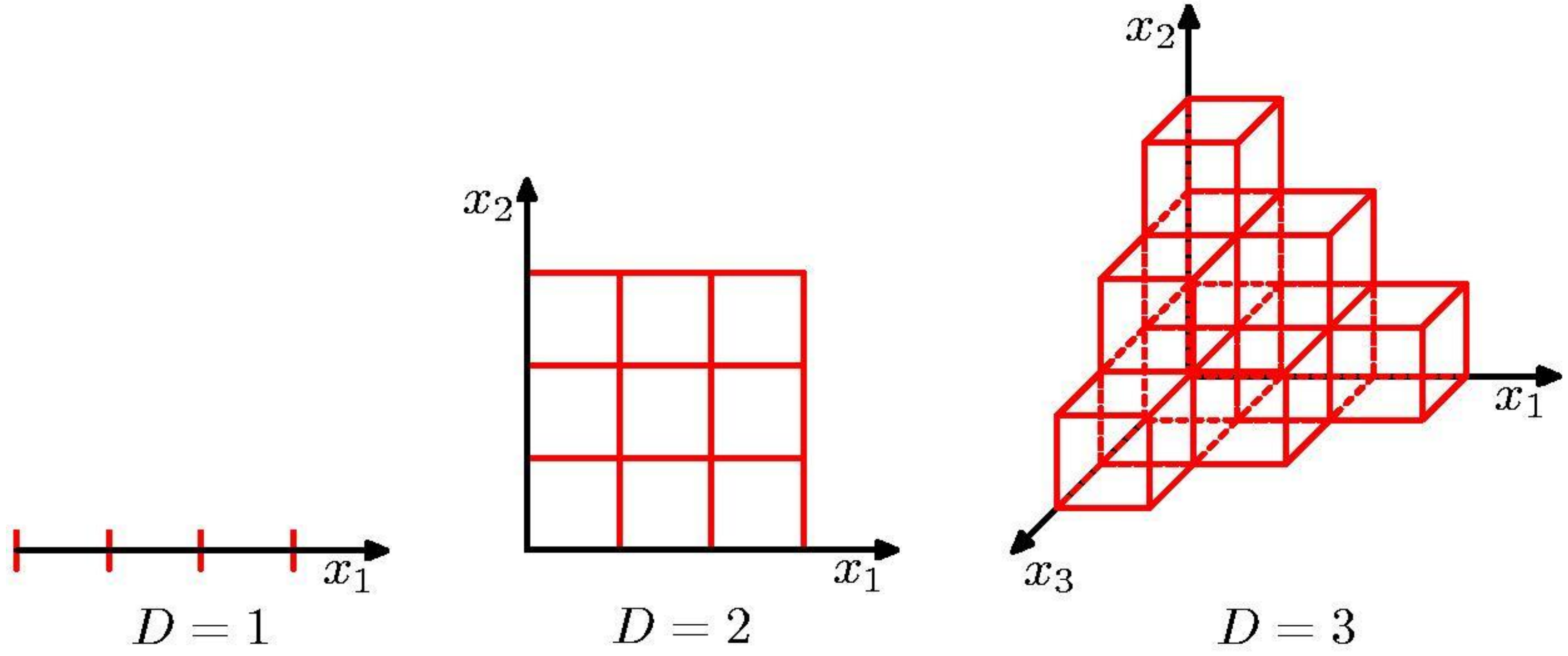
Workflow with Cross-Validation



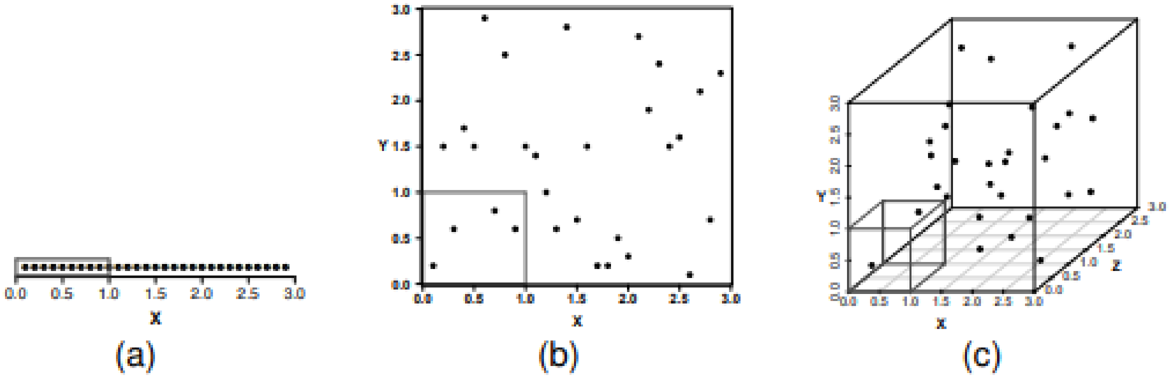
Feature Selection

- A data preprocessing activity usually performed before learning a model.

Curse of Dimensionality



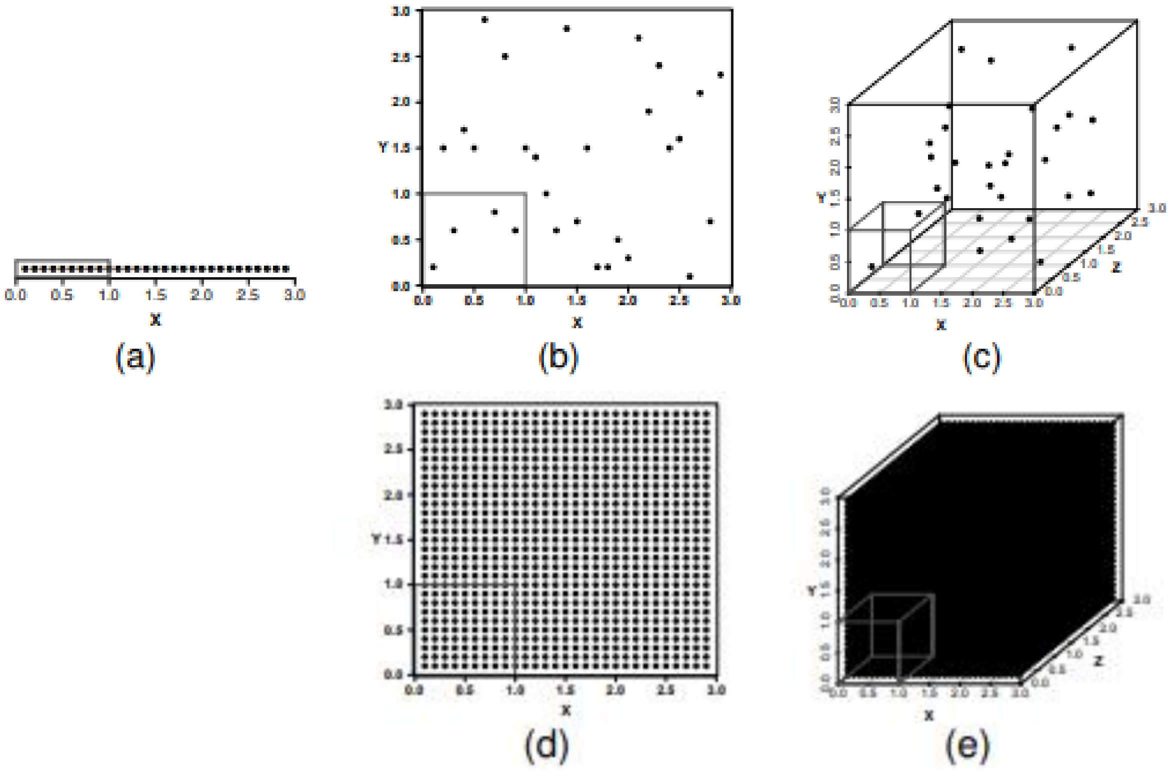
Curse of Dimensionality



(a)
(b)
(c)

Figure: A set of scatter plots illustrating the curse of dimensionality. Across figures (a), (b) and (c) the density of the marked unit hypercubes decreases as the number of dimensions increases.

Curse of Dimensionality



(a) (b) (c)

(d) (e)

Figures (d) and (e) illustrate the cost we must incur if we wish to maintain the density of the instances in the feature space as the dimensionality of the feature space increases.

Feature Selection

- During our discussion of feature selection approaches it will be useful to distinguish between different classes of descriptive features:
  - Predictive
  - Interacting
  - Redundant
  - Irrelevant

Feature Selection

- The search can move through the search space in a number of ways:
  - Forward sequential selection
  - Backward sequential selection

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Machine Learning Tools & Frameworks

Machine Learning Tools & Frameworks

- Python Framework
  - NumPy for numeric computations
  - Pandas for data processing & analysis
  - Matplotlib/Seaborn for visualizations
  - Scikit-learn machine learning library
  - SciPy for scientific computations

  - Anaconda distribution for data driven projects
  - Jupyter notebook
  - VSCode / PyCharm / Spyder (optional)

- Software Packages
  - Knime
  - H2O
  - Node-red
  - …

Introduction to scikit-learn

- https://scikit-learn.org/stable/index.html