Introduction to Machine Learning

Introduction

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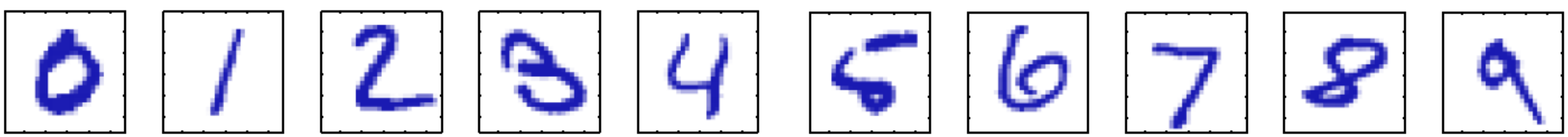
Some slides are modified from Prof. Sheng-Jyh Wang, Prof. Hwang-Tzong Chen, and Prof. Yung-Yu Chuang

Pattern recognition and machine learning

- Pattern recognition is the automated recognition of patterns and regularities in data
  - Discover pattern regularities
  - Take actions, such as classification or regression, with regularities
- Data: A set of hand-written digits and the class ground truth



- Computer algorithm: It extracts features from each image, analyze the patterns and regularities in data
- Model: Given a new hand-written digit, predict its class label

Pattern recognition and machine learning

- Machine learning: to design and develop algorithms that allow computers to predict data based on empirical data
  - Try to explore certain patterns or regularities
  - Learn models from the given data
  - Based on the given data, the learner produces a useful output in new cases
- Machine learning is one approach to pattern recognition, while other approaches include hand-crafted (not learned) rules or heuristics
- Machine learning $\subset$ Pattern recognition

Applications of machine learning

- Computer vision
- Speech recognition
- Information retrieval
- Natural language processing
- Robotics
- Bioinformatics
- Data mining
- Finance
- …

Problem definition of a machine learning task

- Training data
  - A set of N training data $\{\mathbf{x_1}, \mathbf{x_2}, \ldots, \mathbf{x_N}\}$, sometimes together with their target vectors $\{t_1, t_2, \ldots, t_N\}$
- Feature extraction
  - Original input variables are usually transformed into some new space of variables, where the problem can be better handled
- Model learning
  - We learn a proper model for the problem
- Generalization or testing
  - To correctly predict new examples (testing data) that differ from those used for training

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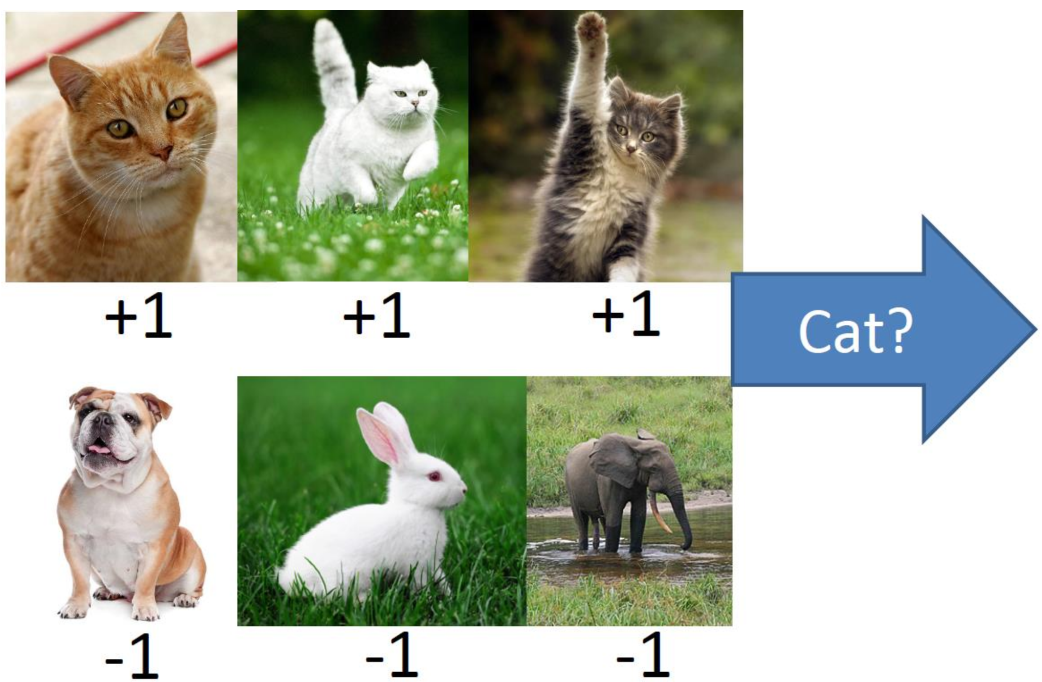
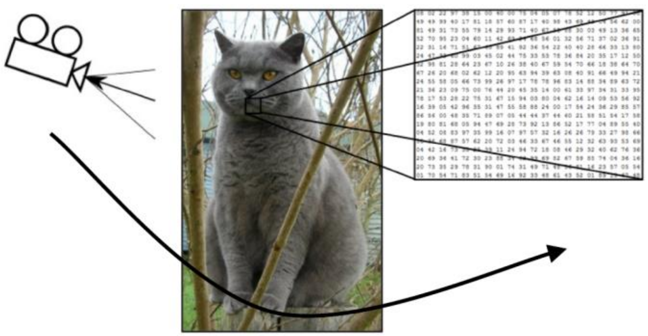
Cat image classification: Training data

- Collect a set of training data with target vectors



Cat image classification: Feature extraction

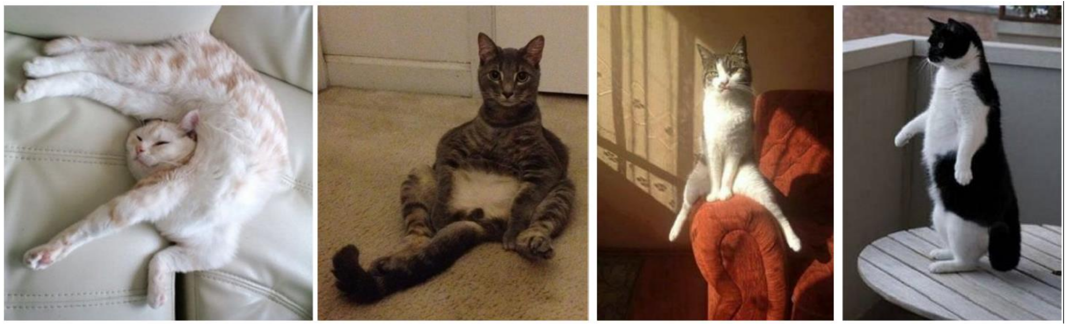
- Feature extraction is crucial
  - Need to take feature variations into account



viewpoint variations

Illumination variations

background variations



pose variations

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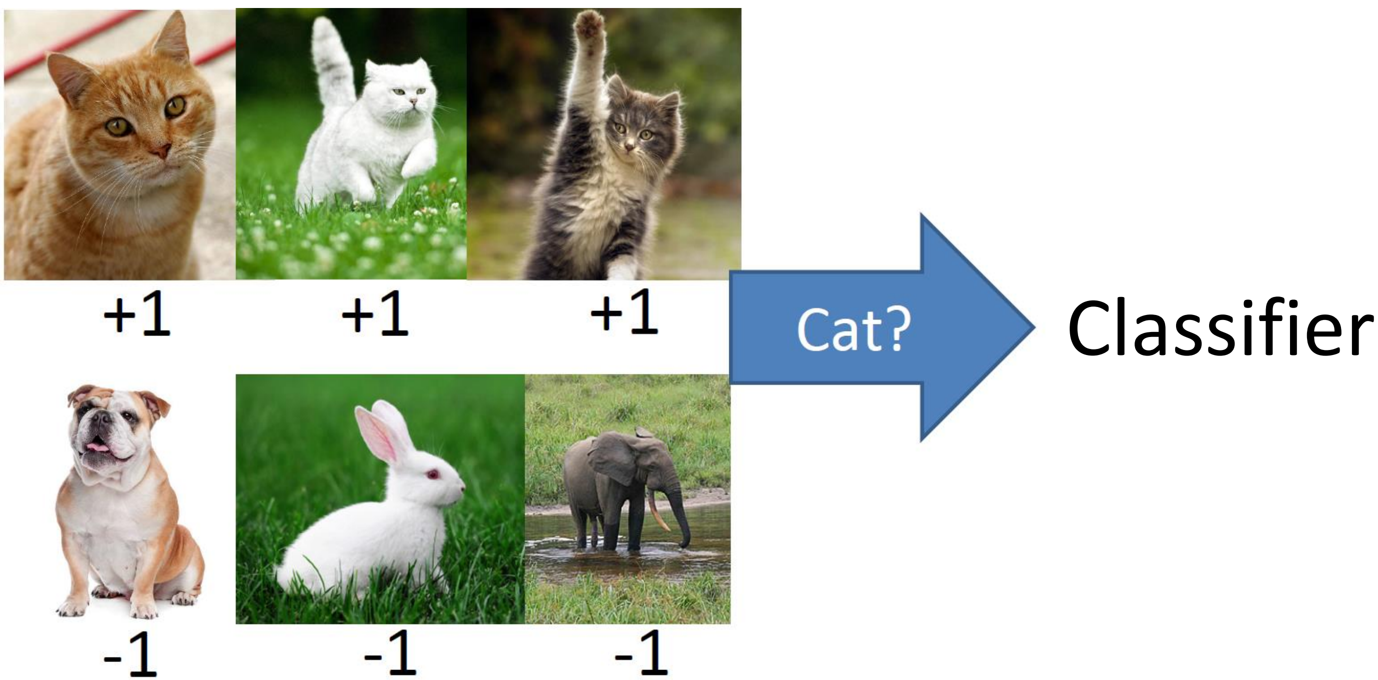
Cat image classification: Model learning

- Based on the given training data and the extracted features, we learn a classifier



Cat image classification: Testing

- Apply the learned classifier to the testing images

Cat image classification: Testing

- Apply the learned classifier to the testing images and make prediction

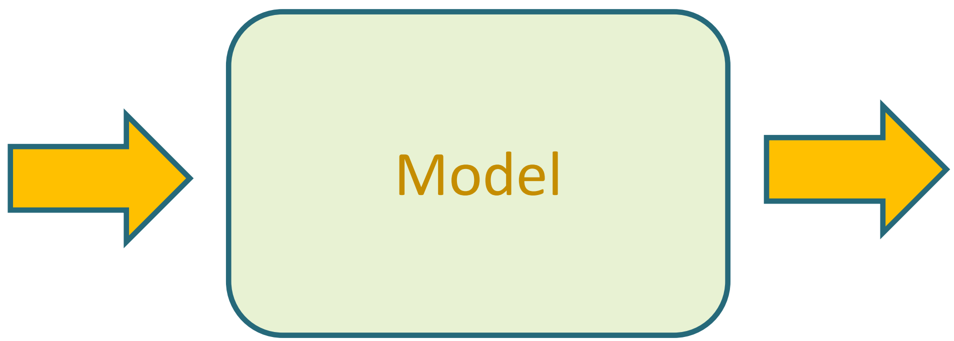
Regression

a real value

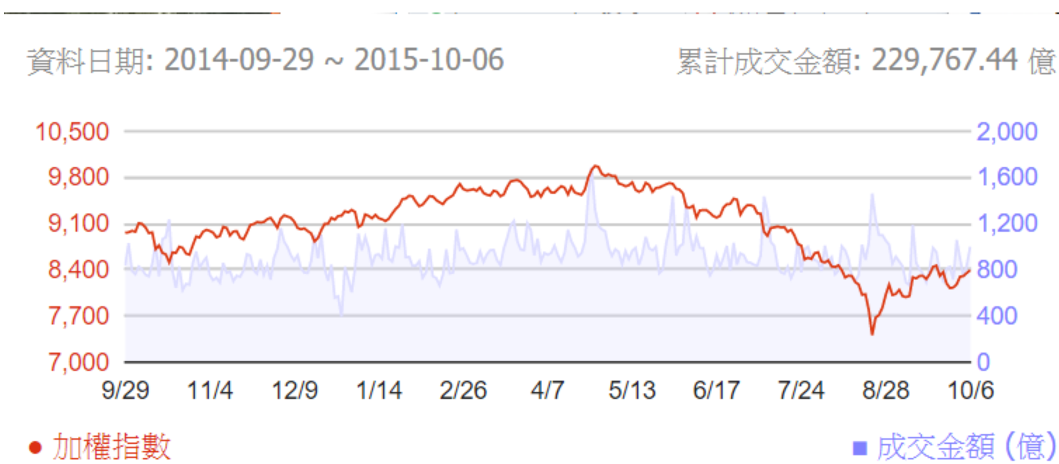
x

y

input data



predicted value



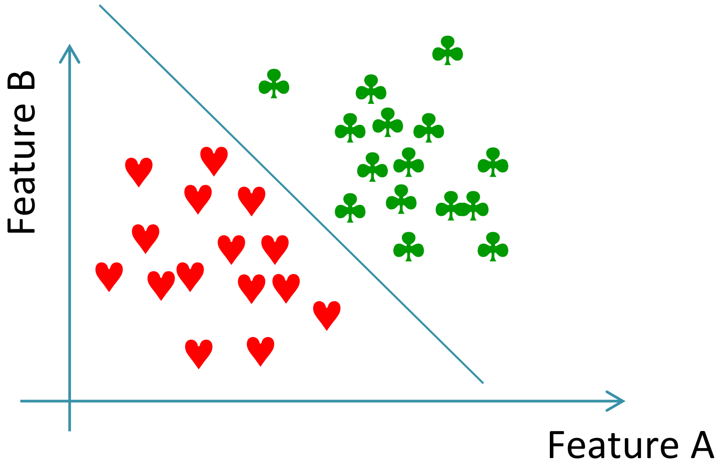
estimated TAIEX on 11/5

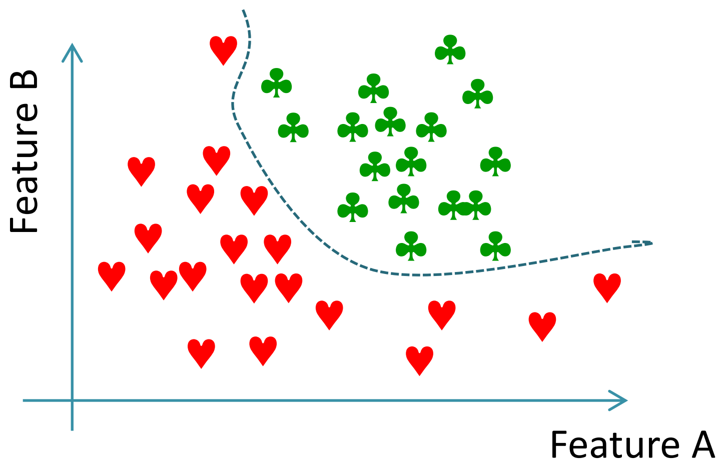
Taiwan Capitalization Weighted Stock Index

Supervised vs. Unsupervised learning

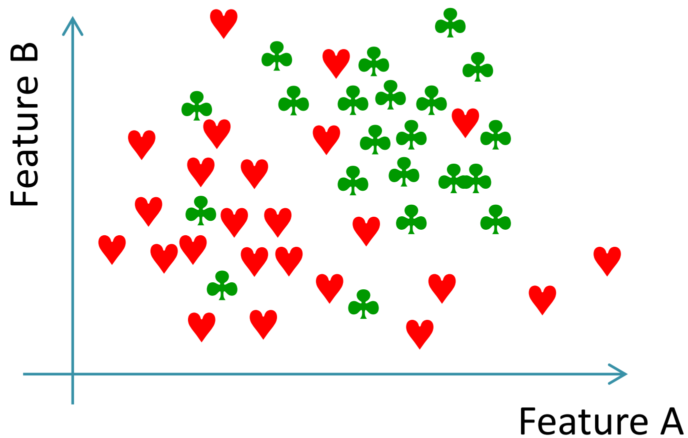
- Supervised learning: the training data comprises examples of the input vectors along with their corresponding target vectors
  - Classification: assign each input vector to one of a finite number of discrete categories
  - Regression: assign each input vector to one or more continuous variables
  - Methods: linear regression, linear classification, neural networks, support vector machine, ensemble learning, dimensionality reduction, deep learning, …

Good vs. bad features for classification



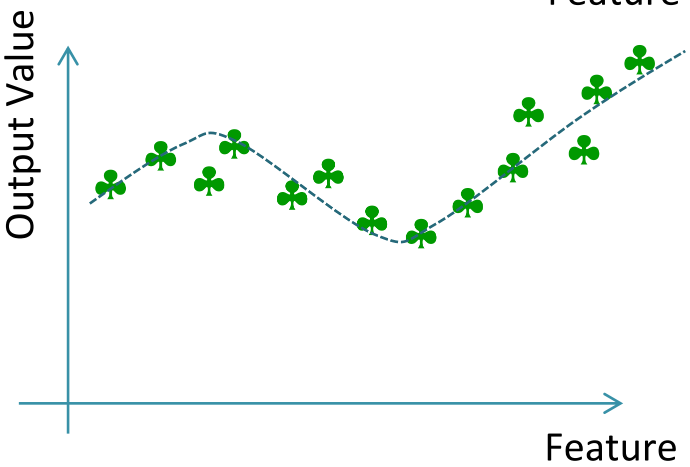


good features

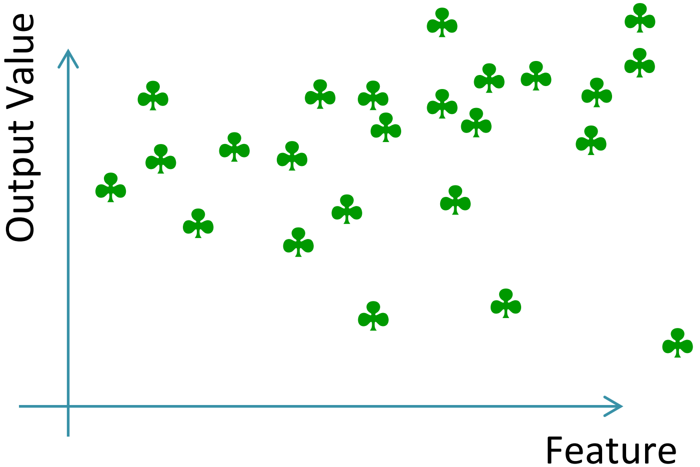


bad features

Good vs. bad features for regression



good feature



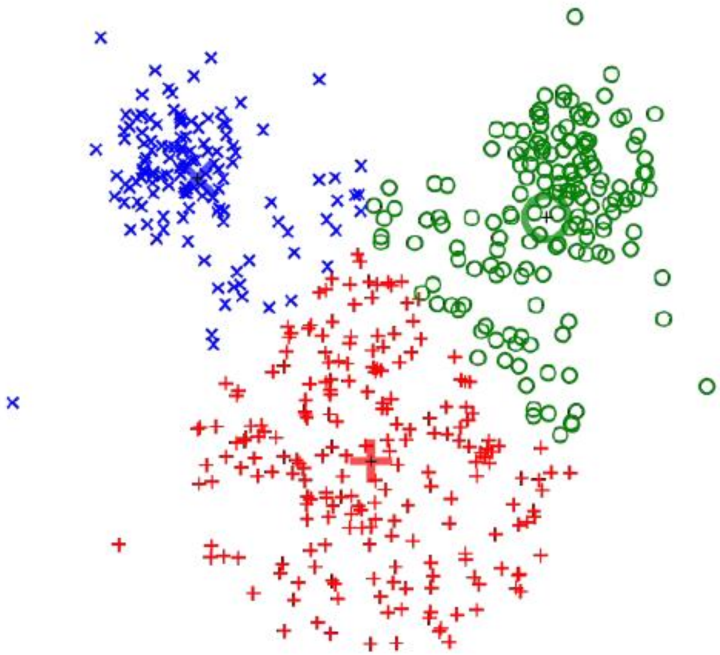
bad feature

Supervised vs. Unsupervised learning

- Unsupervised learning: the training data consist of a set of input vectors x without any corresponding target values
  - Clustering: to discover groups of similar examples within the data
  - Density estimation: to determine the distribution of data within the input space
  - Dimensionality reduction: to project the data from a high-dimensional space down to a low-dimensional space
  - Data generation: to synthesize new data with some particular conditions

Unsupervised learning for clustering

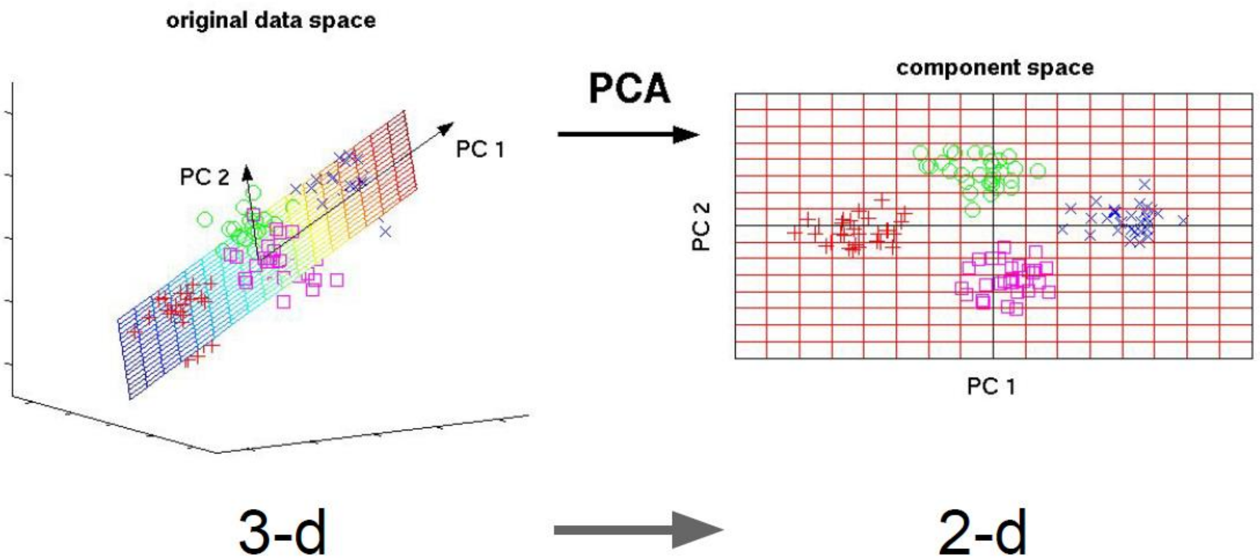
- Clustering: To group a set of data in such a way that data points in the same group, called a **cluster**, are more similar to each other than to those in other clusters



***k*-mean clustering**

Unsupervised learning for dimensionality reduction

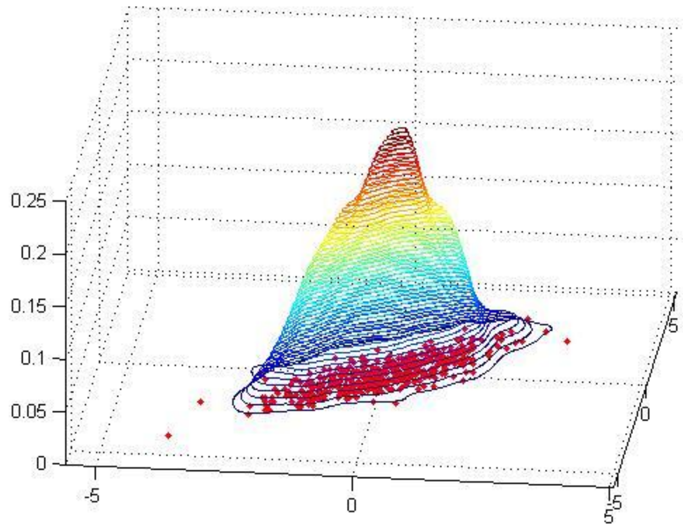
- Dimensionality reduction: To project data from a high-dimensional space to a low-dimensional one



PCA: Principal component analysis

Unsupervised learning for density estimation

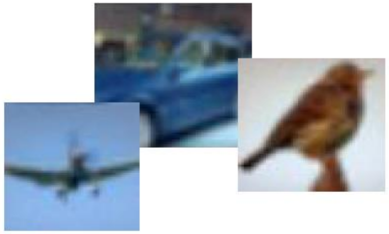
- Density estimation: Based on given data, estimate the underlying probability density function



kernel density estimation (KDE)

Unsupervised learning for data generation

- Given a set of natural images, we try to generate new images that look natural and photorealistic



Training data ~ $p_{data}(x)$

Generated samples ~ $p_{model}(x)$

Generative Adversarial Networks (GAN): Given a set of images, generate new images from the same distributions

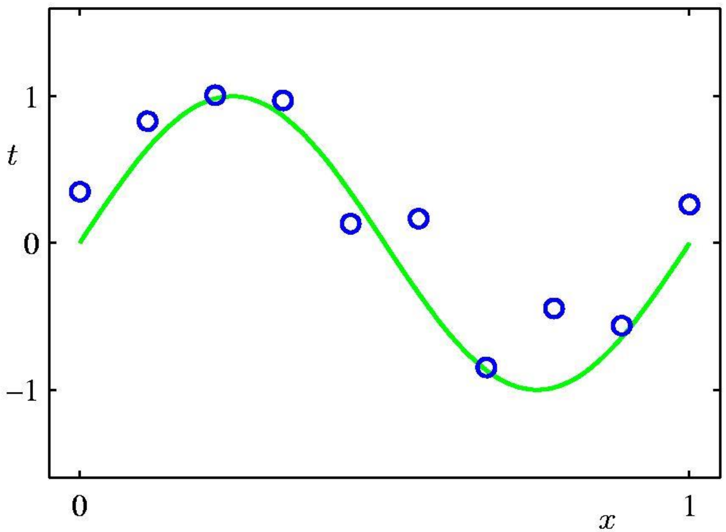
Applications of data generation

- Face synthesis

Tero Karras et al. “Progressive Growing of GANs for Improved Quality, Stability, and Variation”

Polynomial curve fitting: Problem definition

- Training data (observations)
  - 10 blue circles, each of which has
    - One-dimensional input (x-axis)
    - One target output (t-axis)



- Green curve $\sin(2\pi x)$ is the function used to generate these data, which is unknown
- Each point is sampled from the function with a random Gaussian noise
- Goal of curve fitting: To exploit the training data to discover the underlying function so that we can make predictions of the value $\hat{t}$ for some new input $\hat{x}$

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Polynomial curve fitting: Choose a fitting function

- Fit the data using a polynomial function of the form:

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

  - This function is parametrized by **w**
  - w_0 is the bias term
  - Its input is a data point, while the output is estimated target
  - *M* is the order of the polynomial function

Polynomial curve fitting: Error function

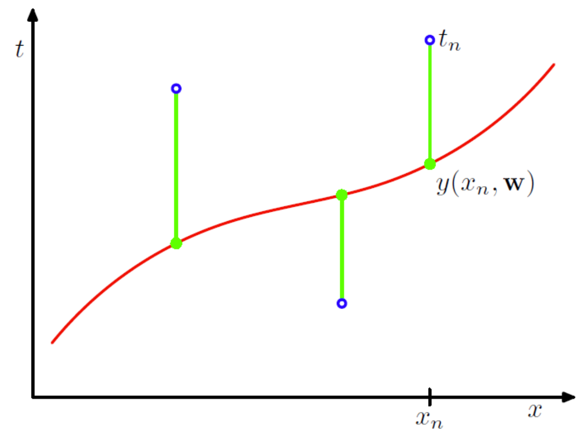
- An error function (objective function) is used to determine the parameters

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

- In this case, we minimize the sum-of-squares error

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

  - Differentiable
  - Closed form solution



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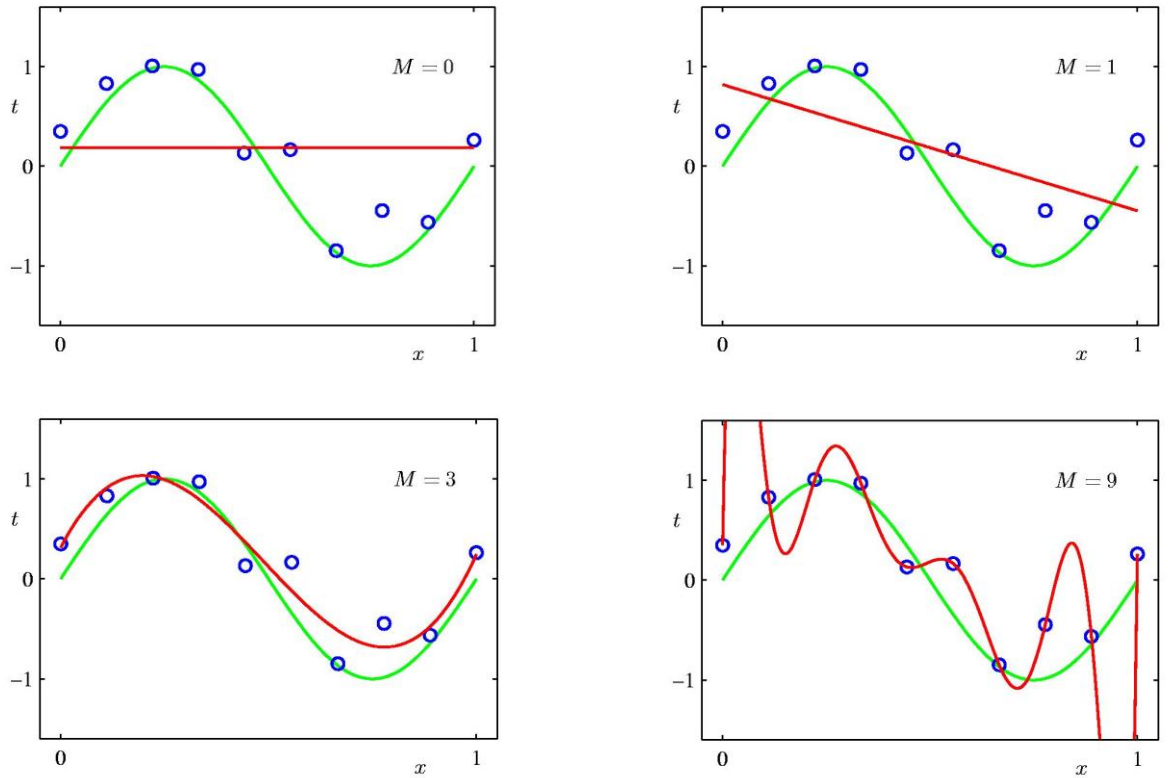
Polynomial curve fitting: Model selection

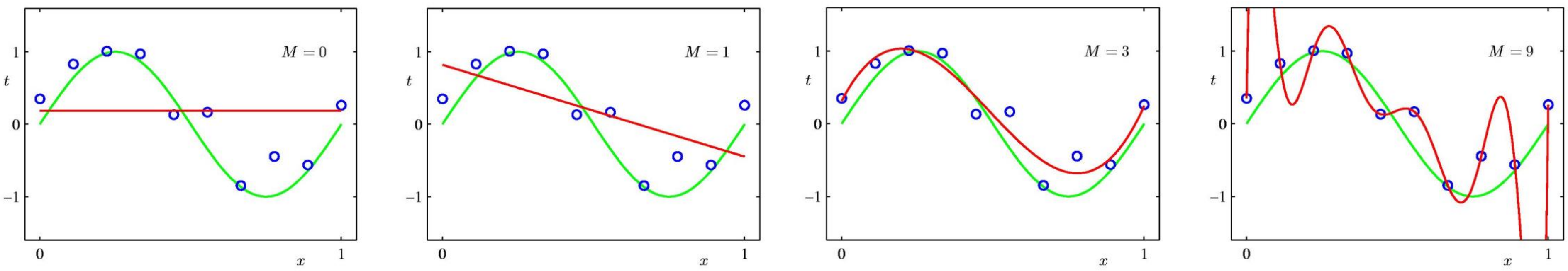
$$y(x, \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + \ldots + w_M x^M = \sum_{j=0}^{M} w_j x^j$$

- Models with different values of hyperparameter *M*



- Model selection: To choose a proper value of *M*

Polynomial curve fitting: Model selection

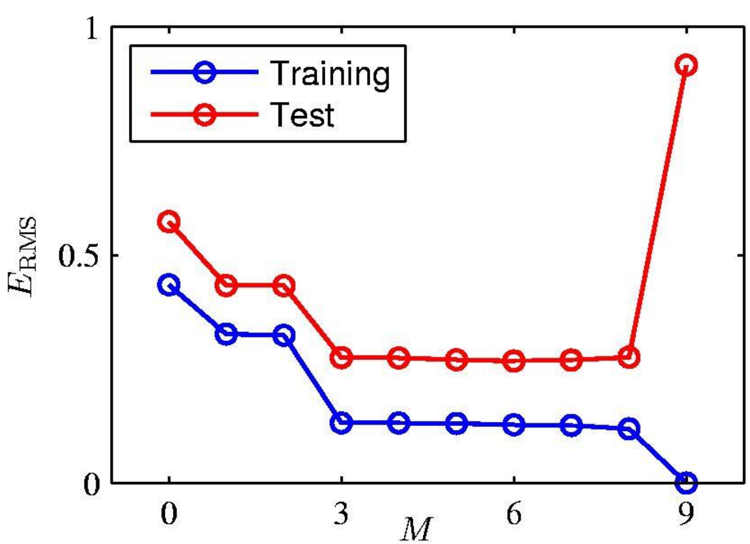


- Under-fitting: M = 0 or M =1
  - The constant or first order polynomial gives poor fit due to insufficient flexibility
- The third order polynomial gives the best fit
- Over-fitting: M = 9
  - All training points are perfectly fitted
  - Poor representation of the green curve
  - The generalization is poor

Polynomial curve fitting: Generalization

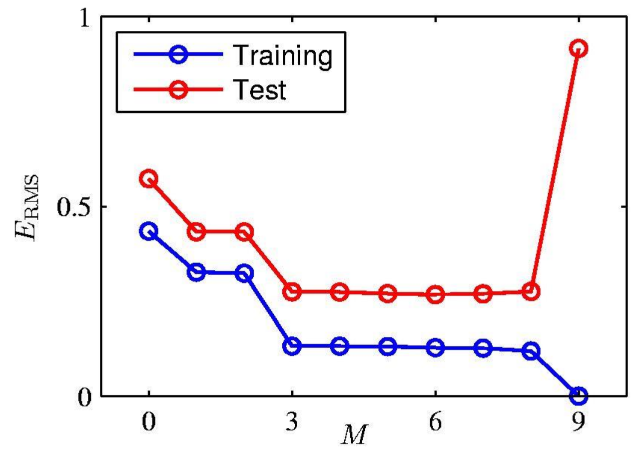
- Suppose we are given a set of training data and a separate set of 100 test data
- Evaluate the generalization for each choice of *M* via root-mean-square (RMS) error

$$E_{\mathrm{RMS}} = \sqrt{2E(\mathbf{w}^\star)/N}$$



	$M = 0$	$M = 1$	$M = 3$	$M = 9$
$w_0^\star$	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

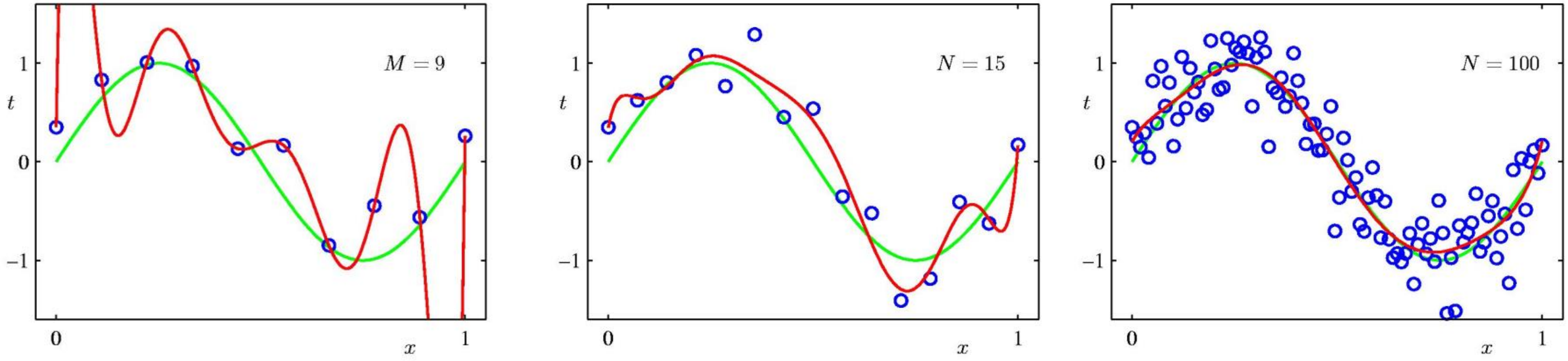
Polynomial curve fitting: Generalization



- Small values of *M* give relatively large values of training and test errors
- When *M* is between 3 and 8, reasonable representations are obtained
- For *M*=9, the training error goes to zero, but the test error increases significantly

Polynomial curve fitting: Data size vs. Over-fitting

$M = 9$



- Over-fitting becomes less severe as the data size increases
- In general, the number of data points should be no less than some multiple (say 5 or 10) of the number of adaptive parameters in the model
- Regularization is often used to control the over-fitting phenomenon

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Polynomial curve fitting: Regularization

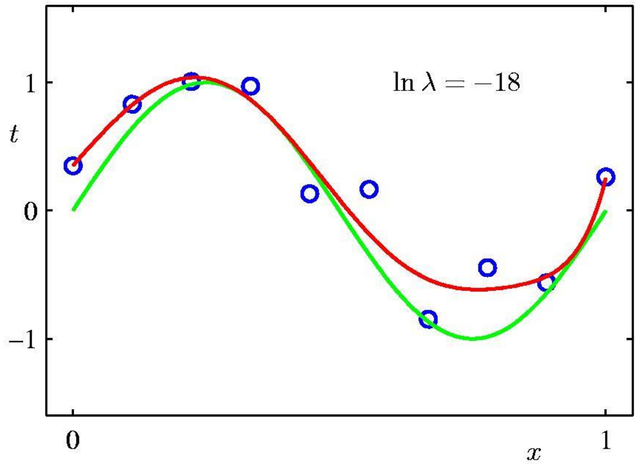
- Regularization: Add a penalty term to the error function to discourage the coefficients from reaching large values

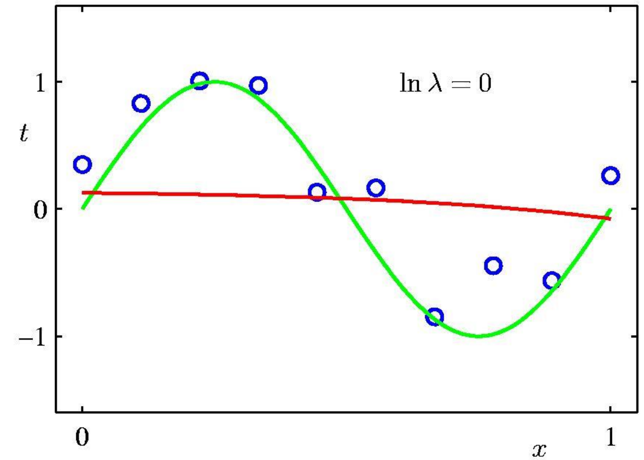
$$\widetilde{E}(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(x_n, \mathbf{w}) - t_n\}^2 + \frac{\lambda}{2}\|\mathbf{w}\|^2$$

where $\|\mathbf{w}\|^2 = \mathbf{w}^T\mathbf{w} = \omega_0^2 + \omega_1^2 + \cdots + \omega_M^2$

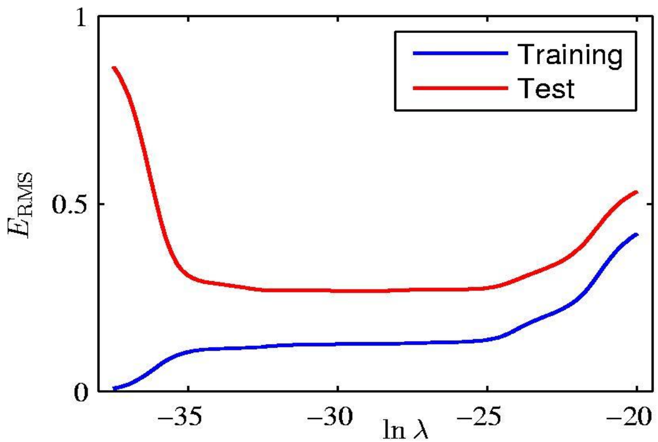
  - The coefficient ω_0 is usually omitted
  - This kind of techniques is called shrinkage methods in the statistics literature
  - A quadratic regularizer is called ridge regression
  - In neural networks, this approach is known as weight decay

Polynomial curve fitting: Regularization





	$\ln \lambda = -\infty$	$\ln \lambda = -18$	$\ln \lambda = 0$
$w_0^\star$	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

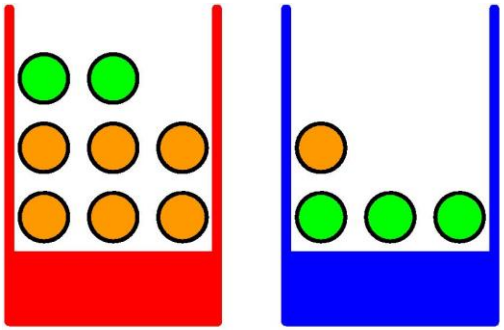


Probability theory

- We need to handle data uncertainties, which result from
  - Noise on measurement
  - Finite size of data sets

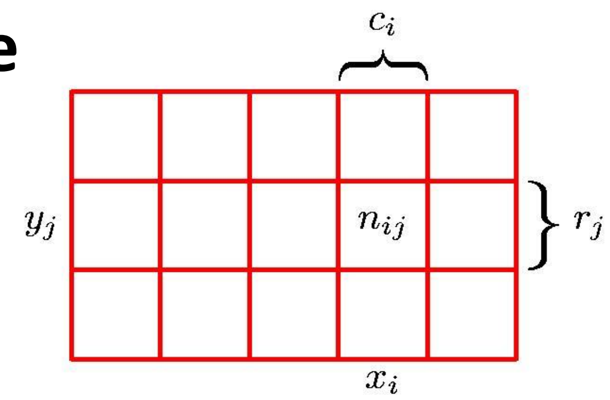
- Probability theory provides a consistent framework to manipulate uncertainties, and hence is essential to pattern recognition research

A toy example



- Two boxes: *r* (red box) and *b* (blue box)
- Two types of fruits: *a* (apple) and *o* (orange)
- A trial: Randomly selecting a box from which we randomly picking a fruit
- Introduce one variable *B* for box and one variable *F* for fruit
- Many trials: Repeat the process many times
- Question 1: What is the probability that an apple is picked
  - Marginal probability
- Question 2: Given that we have picked an orange, what is the probability that the box we chose was the blue one?
  - Conditional probability

Probability theory: A two-variable case



- Two random variables: X and Y
- Each variable has a set of discrete states
  - X can take any value x_i where $i = 1, 2, \ldots, M$
  - Y can take any value y_j where $j = 1, 2, \ldots, L$
- N trails where both variables X and Y are sampled
- Some notations
  - Let the number of trails where $X = x_i$ and $Y = y_j$ be n_{ij}
  - Let the number of trails where X takes value x_i be c_i
  - Let the number of trails where Y takes value y_j be r_j

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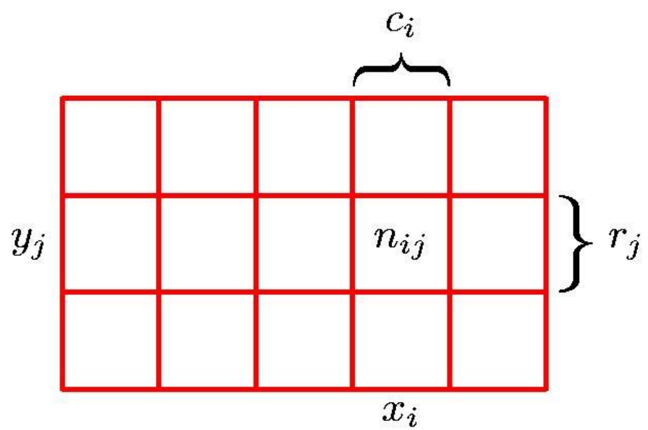
Joint, marginal, and conditional probabilities



- The probability that X takes value x_i and Y takes value y_j is called joint probability

- It is defined by the fraction of points (trails) falling in the cell *i,j*

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

Joint, marginal, and conditional probabilities

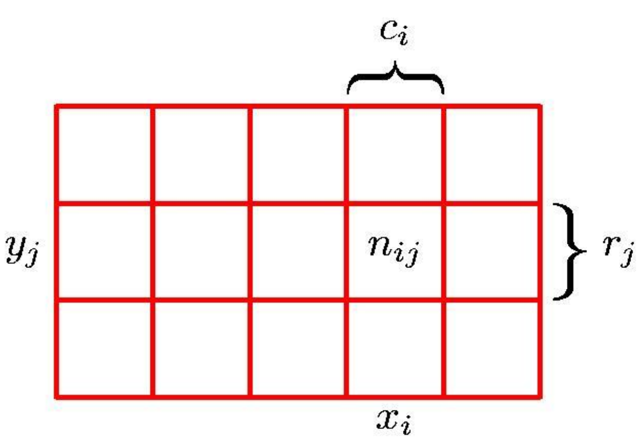
- The probability that X takes value x_i irrespective of the value of Y is called marginal probability and is written as $p(X = x_i)$

- It is defined by the fraction of the number of points that fall in column *i*, namely

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

- With the joint probability and $c_i = \sum_j n_{ij}$, we have

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



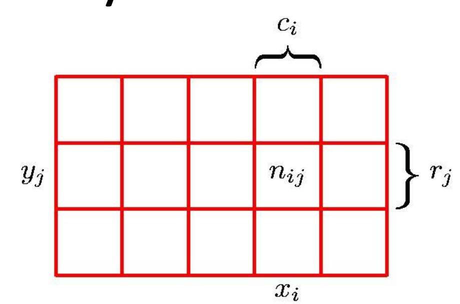
- The sum rule

Joint, marginal, and conditional probabilities

- If we consider only those cases where X takes value x_i, the fraction of those cases where $Y = y_j$ is written as $p(Y = y_j | X = x_i)$. It is called conditional probability

- It is defined by

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



- Relationships among joint, marginal, and conditional probabilities:

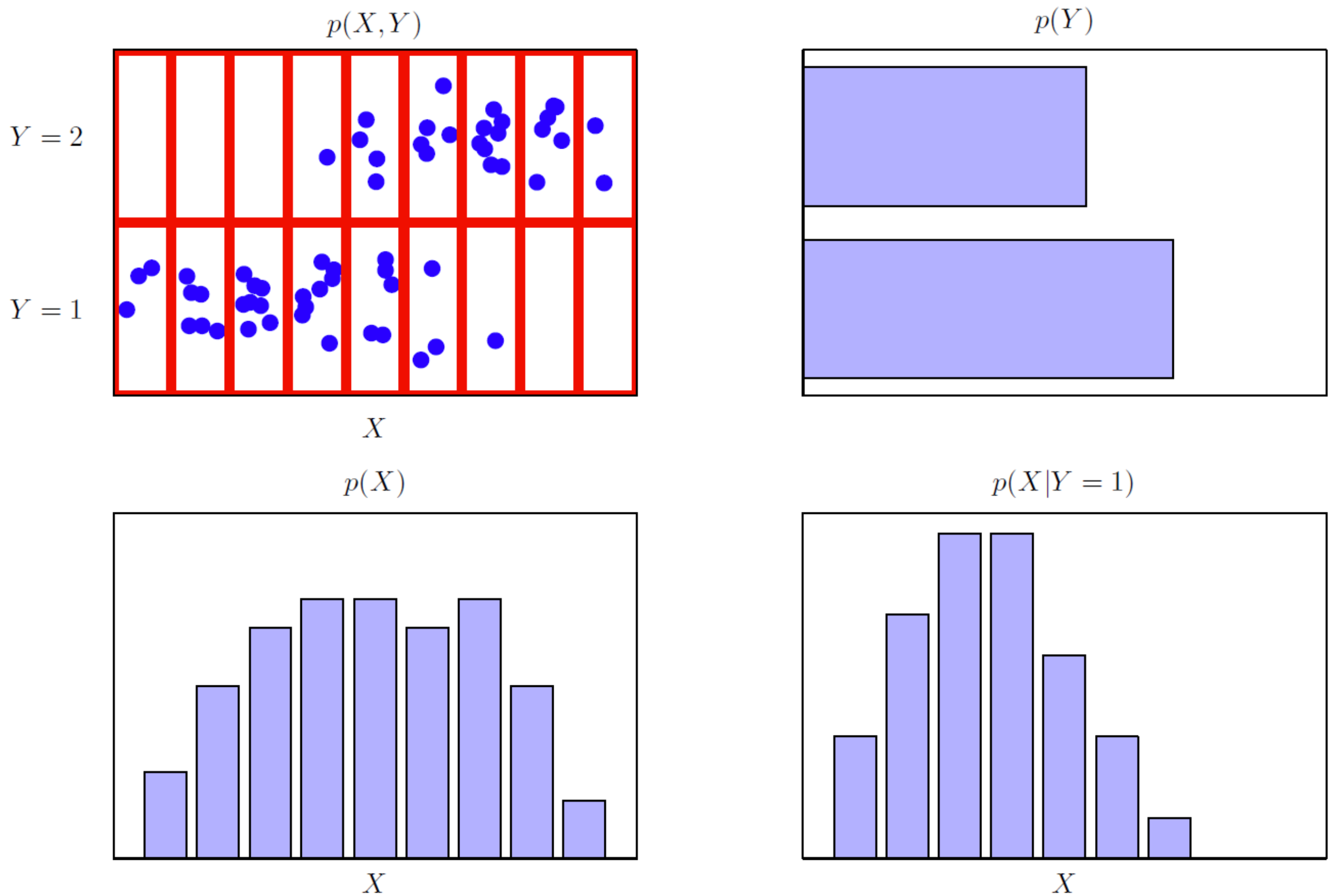
$$\begin{aligned} p(X = x_i, Y = y_j) &= \frac{n_{ij}}{N} = \frac{n_{ij}}{c_i} \cdot \frac{c_i}{N} \\ &= p(Y = y_j | X = x_i) p(X = x_i) \end{aligned}$$

- The product rule

Joint, marginal, and conditional probabilities

sum rule $$p(X) = \sum_Y p(X, Y)$$

product rule $$p(X, Y) = p(Y|X)p(X)$$



Bayes' theorem

- By using the product rule and the symmetry property $p(X,Y)$=$p(Y,X)$, we have

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

Probability with continuous variables

- The probability density $p(x)$ over a continuous variable x must satisfy the two conditions:

$$p(x) \geqslant 0$$

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

  - Nonnegative: Probabilities are nonnegative
  - Sum-to-1: The value of x must lie somewhere on the real axis

- The cumulative distribution function defines the probability that x lies in the interval $(-\infty, z)$ via

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

Sum rule and product rule

- Sum rule in discrete cases

$$p(X) = \sum_Y p(X, Y)$$

- Sum rule in continuous cases

$$p(x) \quad = \quad \int p(x, y) \, \mathrm{d}y$$

- Product rule in discrete cases

$$p(X, Y) = p(Y|X)p(X)$$

- Product rule in continuous cases

$$p(x, y) \quad = \quad p(y|x)p(x)$$

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Expectations and covariances

- The average value of some function $f(x)$ under a probability distribution $p(x)$ is called the expectation of $f(x)$

- For a discrete distribution, the expectation of $f(x)$ is

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

- For a continuous probability, the expectation of $f(x)$ is

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

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Expectations and covariances

- The variance of $f(x)$ under a probability distribution $p(x)$ is

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

- It is a measure of how much variability there is in $f(x)$ around its mean $\mathbb{E}[f(x)]$

- For two random variables x and y, the covariance is defined by

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

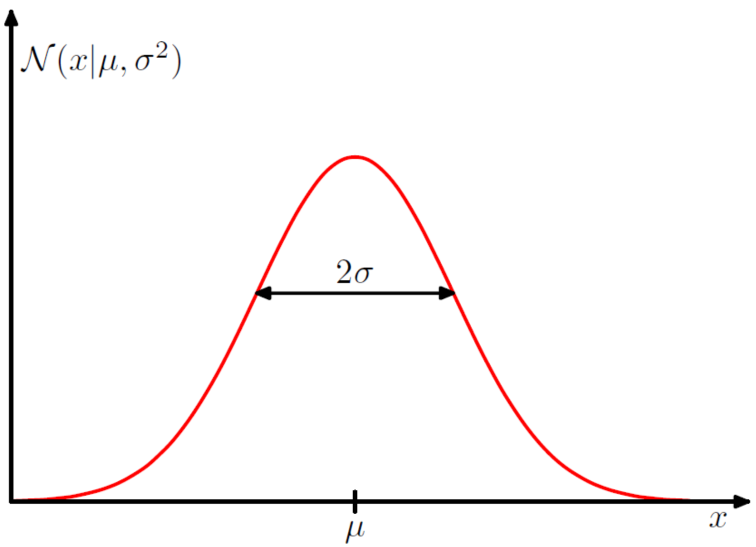
- It expresses the extent to which x and y vary together.

Gaussian distribution

- For a single continuous variable, the Gaussian or normal distribution is defined by

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

which is specified by two parameters: mean μ and variance σ^2



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

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

Mean and variance of a Gaussian distribution

- The average value of a random variable x whose distribution is Gaussian

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

- The second order moment of variable x

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

- The variance of variable x

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

Multivariate Gaussian

- The multivariate Gaussian distribution defined over a *D*-dimensional vector **x** of continuous variables:

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

where *D* x *D* matrix is called the co-variance matrix while $|\boldsymbol{\Sigma}|$ denotes the determinant of $\boldsymbol{\Sigma}$

Bayes' theorem for polynomial curve fitting

- Recall the curve fitting problem
  - Given a set of *N* observations *D* = {$\mathbf{x}_1$, $\mathbf{x}_2$, …, $\mathbf{x}_N$} and their target values {t_1, t_2, …, t_N}
  - Polynomial curve fitting: Determine the values of $\boldsymbol{w}$

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

- Prior probability $p(\boldsymbol{w})$: Express our assumption about $\boldsymbol{w}$ before observing any data
- Likelihood function $p(D|\boldsymbol{w})$: Express how probable the observed data *D* is under $\boldsymbol{w}$. It is evaluated after the observations *D* are given

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Bayes' theorem for polynomial curve fitting

- Bayes' theorem takes the form

$$p(\mathbf{w}|\mathcal{D}) = \frac{p(\mathcal{D}|\mathbf{w})p(\mathbf{w})}{p(\mathcal{D})}$$

  which allows us to evaluate the uncertainty after we have observations *D*

- $p(D)$ is the normalization constant. Thus, we have

$$\text{posterior} \;\propto\; \text{likelihood} \;\times\; \text{prior}$$

Determining Gaussian parameters by maximum likelihood

- Given a set of *N* observations: $\mathbf{x} = (x_1, \ldots, x_N)$
- Assume these observations are sampled from a Gaussian distribution with mean μ and variance σ^2 (unknown)
- Our goal is to determine μ and σ^2 based on the observations
- We assume that data are sampled independently from the same distribution, namely independent and identically distributed, or i.i.d. for short

Determining Gaussian parameters by maximum likelihood

- Since the data are i.i.d., the likelihood function of data given mean μ and variance σ^2 is

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

- The log likelihood function is

$$\ln p\left(\mathbf{x}|\mu, \sigma^2\right) = -\frac{1}{2\sigma^2}\sum_{n=1}^{N}(x_n - \mu)^2 - \frac{N}{2}\ln\sigma^2 - \frac{N}{2}\ln(2\pi)$$

- Maximum likelihood solution:

$$\mu_{\mathrm{ML}} = \frac{1}{N}\sum_{n=1}^{N} x_n \qquad \sigma^2_{\mathrm{ML}} = \frac{1}{N}\sum_{n=1}^{N}(x_n - \mu_{\mathrm{ML}})^2$$

Probabilistic perspective of polynomial curve fitting

- Given *N* data for regression: $\mathbf{x} = (x_1, \ldots, x_N)^{\mathrm{T}}$ & $\mathbf{t} = (t_1, \ldots, t_N)^{\mathrm{T}}$
  - Fit the data using a polynomial function of the form:

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

  - This function is parametrized by $\mathbf{w}$

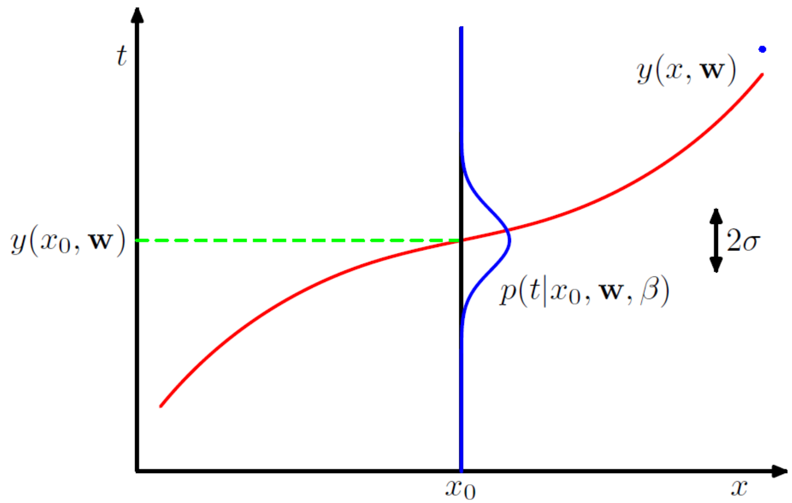
- Given the value of x, we assume the corresponding value of t has a Gaussian distribution with a mean equal to $y(x, \boldsymbol{w})$

$$p(t|x, \mathbf{w}, \beta) = \mathcal{N}\left(t|y(x, \mathbf{w}), \beta^{-1}\right)$$

where β^{-1} is the variance σ^2 (β is called precision)

Probabilistic perspective of polynomial curve fitting

- The Gaussian conditional distribution for t given x



- If data are i.i.d., the likelihood function is

$$p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta) = \prod_{n=1}^{N} \mathcal{N}\left(t_n | y(x_n, \mathbf{w}), \beta^{-1}\right)$$

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Maximum likelihood solution

- The log likelihood function

$$\ln p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta) = -\frac{\beta}{2}\sum_{n=1}^{N}\{y(x_n, \mathbf{w}) - t_n\}^2 + \frac{N}{2}\ln\beta - \frac{N}{2}\ln(2\pi)$$

- Maximum likelihood (ML) solution for determining $\mathbf{w}$ and β
  - Compute the gradient of the log likelihood function w.r.t. $\mathbf{w}$. And set it to 0. We can get $\mathbf{w}_{\mathrm{ML}}$

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

  - By setting the gradient of the log likelihood function w.r.t. β to 0, β_{ML} is obtained by solving

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

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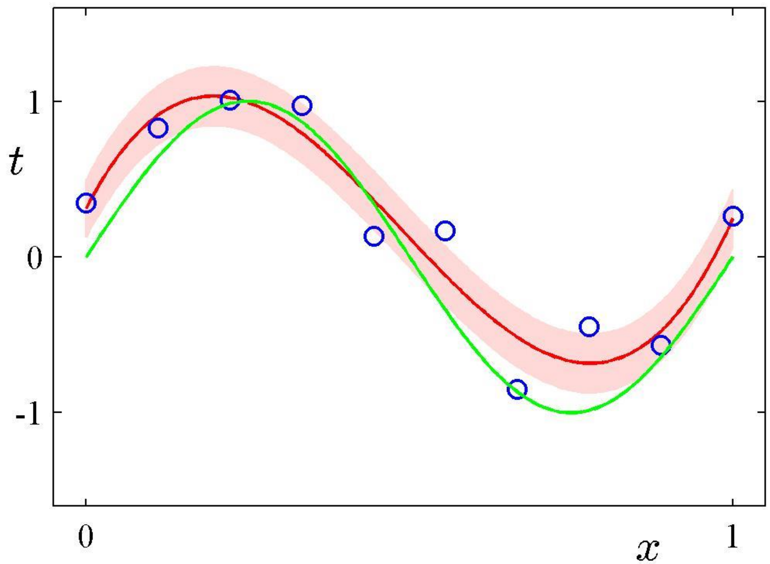
Maximum likelihood solution

- After determining the values of $\mathbf{w}_{\mathrm{ML}}$ and β_{ML}, we can make predictions for a new value of x

$$p(t|x, \mathbf{w}_{\mathrm{ML}}, \beta_{\mathrm{ML}}) = \mathcal{N}\left(t|y(x, \mathbf{w}_{\mathrm{ML}}), \beta_{\mathrm{ML}}^{-1}\right)$$



Maximum a posterior (MAP) solution

- While ML solution is obtained by maximizing the likelihood, MAP solution is by maximizing the posterior
- Recall $\text{posterior} \propto \text{likelihood} \times \text{prior}$
- Introduce a prior distribution over the curve parameters $\mathbf{w}$

$$p(\mathbf{w}|\alpha) = \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}) = \left(\frac{\alpha}{2\pi}\right)^{(M+1)/2} \exp\left\{-\frac{\alpha}{2}\mathbf{w}^{\mathrm{T}}\mathbf{w}\right\}$$

  - M is the order of the polynomial
  - α is a hyperparameter
- The posterior distribution for $\mathbf{w}$

$$p(\mathbf{w}|\mathbf{x}, \mathbf{t}, \alpha, \beta) \propto p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta)p(\mathbf{w}|\alpha).$$

Maximum a posterior (MAP) solution

- The MAP solution, $\mathbf{w}_{\mathrm{MAP}}$ and β_{MAP}, is obtained by maximizing the posterior function, or equivalently by minimizing

$$\frac{\beta}{2}\sum_{n=1}^{N}\{y(x_n,\mathbf{w})-t_n\}^2+\frac{\alpha}{2}\mathbf{w}^{\mathrm{T}}\mathbf{w}.$$

Bayesian curve fitting

- We make a point estimation of $\mathbf{w}$ no matter in ML and MAP solutions
- In a full Bayesian approach, we integrate over all possible values of $\mathbf{w}$ for regression, i.e.,

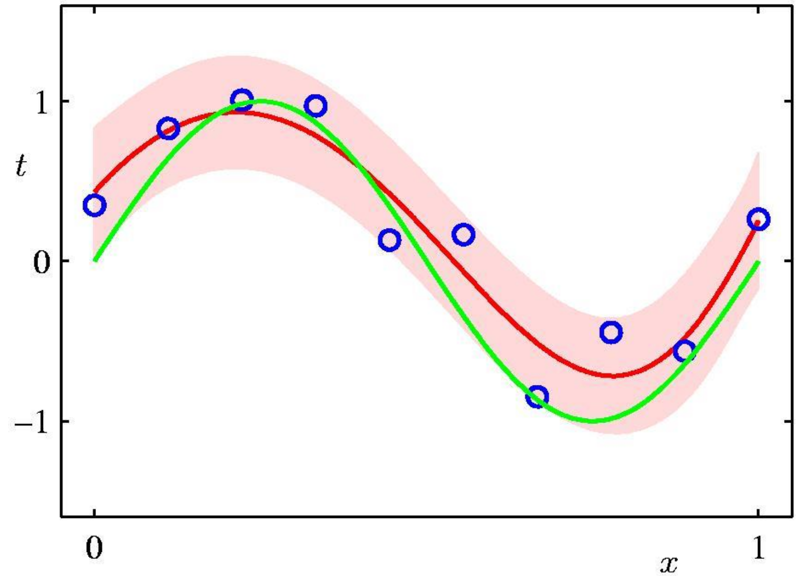
$$p(t|x,\mathbf{x},\mathbf{t}) = \int p(t|x,\mathbf{w})p(\mathbf{w}|\mathbf{x},\mathbf{t})\,\mathrm{d}\mathbf{w} = \mathcal{N}\left(t|m(x), s^2(x)\right)$$

$$m(x) = \beta\boldsymbol{\phi}(x)^{\mathrm{T}}\mathbf{S}\sum_{n=1}^{N}\boldsymbol{\phi}(x_n)t_n$$

$$s^2(x) = \beta^{-1} + \boldsymbol{\phi}(x)^{\mathrm{T}}\mathbf{S}\boldsymbol{\phi}(x).$$

$$\phi(x_n) = (x_n^0, \ldots, x_n^M)^T$$

$$\mathbf{S}^{-1} = \alpha\mathbf{I} + \beta\sum_{n=1}^{N}\boldsymbol{\phi}(x_n)\boldsymbol{\phi}(x)^{\mathrm{T}}$$



Probabilistic polynomial curve fitting

- Given the assumption $p(t|x, \mathbf{w}, \beta) = \mathcal{N}\left(t|y(x, \mathbf{w}), \beta^{-1}\right)$
  - ML solution: Find **w** that maximizes the likelihood function

$$p(t \mid x, D) = p(t \mid x, \mathbf{w}_{\mathbf{ML}}, \beta^{-1})$$

  - MAP solution: Find **w** that maximizes the posterior probability

$$p(t \mid x, D) = p(t \mid x, \mathbf{w}_{\mathbf{MAP}}, \beta^{-1})$$

  - Bayesian solution: Integrate over **w**

$$p(t \mid x, D) = p(t|x, \mathbf{x}, \mathbf{t}) = \int p(t|x, \mathbf{w}) p(\mathbf{w}|\mathbf{x}, \mathbf{t}) \, \mathrm{d}\mathbf{w}$$

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Model selection

- Hyperparameters, such as M in polynomial curve fitting, control the model behavior complexity

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

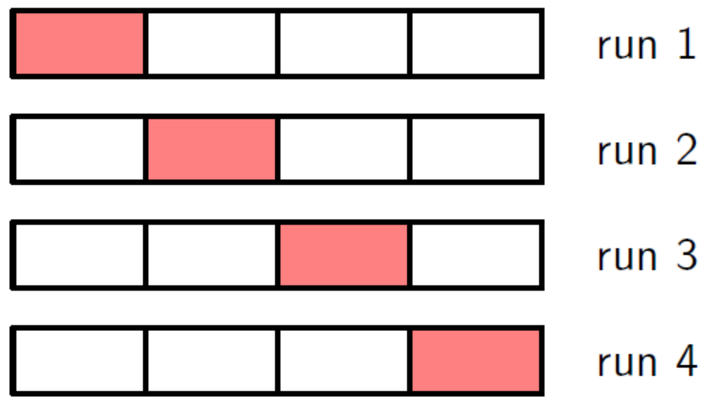
- Model selection: determine the values of hyperparameters that achieve the best predictive performance on new (testing) data
- Idea: split training data into a training set and a validation set
  - Training set: Used to learn the model with particular hyperparameter values
  - Validation set: Used to evaluate the performance of the learned model

Model selection

- About the size of the validation set
  - A large validation set: Less training data for model learning
  - A small validation set: Less reliable performance evaluation

Model selection via cross validation

- *S*-fold cross-validation
  - Partition training data into *S* equal-sized groups
  - *S*-1 groups are used to train the model that is evaluated on the remaining group
  - Repeat the procedure for all *S* possible runs
  - Average the performance



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Drawbacks of model selection

- If training data are limited, a large value of S is appropriate
- At the extreme, setting $S=N$ (number of training data), it gives the leave-one-out technique
- Some drawbacks
  - ➢ The number of training runs increases by a factor of S
  - ➢ The number of hyperparameter value combinations increases exponentially

Summary

- Polynomial curve fitting for regression
  - Fitting by minimizing the sum-of-squares error

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

  - Regularization for alleviating overfitting

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

- Probability density
  - Expectation, variance, and covariance
  - Gaussian distribution

Summary

- Bayes' theorem

$$\text{posterior} \propto \text{likelihood} \times \text{prior}$$

- When applying Bayes' theorem to polynomial curve fitting,
  - ML solution: Find $\mathbf{w}$ that maximizes the likelihood function
  - MAP solution: Find $\mathbf{w}$ that maximizes the posterior probability
  - Bayesian solution: Integrate over $\mathbf{w}$
- Model selection by cross-validation

References

- Chapters 1.1, 1.2, 1.3, and 1.4 in the PRML textbook

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Thank You for Your Attention!

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