Probability Theory for Machine Learning

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September 2015

Outline

- Motivation
- Probability Definitions and Rules
- Probability Distributions
- MLE for Gaussian Parameter Estimation
- MLE and Least Squares
- Least Squares Demo

Material

- Pattern Recognition and Machine Learning - Christopher M. Bishop
- All of Statistics – Larry Wasserman
- Wolfram MathWorld
- Wikipedia

Motivation

- Uncertainty arises through:
  - Noisy measurements
  - Finite size of data sets
  - Ambiguity: The word bank can mean (1) a financial institution, (2) the side of a river, or (3) tilting an airplane. Which meaning was intended, based on the words that appear nearby?
  - Limited Model Complexity
- Probability theory provides a consistent framework for the quantification and manipulation of uncertainty
- Allows us to make optimal predictions given all the information available to us, even though that information may be incomplete or ambiguous

Sample Space

- The sample space Ω is the set of possible outcomes of an experiment. Points ω in Ω are called sample outcomes, realizations, or elements. Subsets of Ω are called Events.

- Example. If we toss a coin twice then $\Omega = \{HH, HT, TH, TT\}$. The event that the first toss is heads is $A = \{HH, HT\}$

- We say that events A1 and A2 are disjoint (mutually exclusive) if $Ai \cap Aj = \{\}$
  - Example: first flip being heads and first flip being tails

Probability

- We will assign a real number P(A) to every event A, called the probability of A.
- To qualify as a probability, P must satisfy three axioms:
  - Axiom 1: $P(A) \geq 0$ for every A
  - Axiom 2: $P(\Omega) = 1$
  - Axiom 3: If A1,A2, . . . are disjoint then

$$\mathbb{P}\left(\bigcup_{i=1}^{\infty} A_i\right) = \sum_{i=1}^{\infty} \mathbb{P}(A_i)$$

Joint and Conditional Probabilities

- Joint Probability
  - $P(X,Y)$
  - Probability of X and Y

- Conditional Probability
  - $P(X|Y)$
  - Probability of X given Y

Independent and Conditional Probabilities

- Assuming that P(B) > 0, the **conditional** probability of A given B:
- $P(A|B)=P(AB)/P(B)$
- $P(AB) = P(A|B)P(B) = P(B|A)P(A)$
  - Product Rule

- Two events A and B are **independent** if
- $P(AB) = P(A)P(B)$
  - Joint = Product of Marginals

If disjoint, are events A and B also independent?

- Two events A and B are **conditionally independent** given C if they are independent after conditioning on C
- $P(AB|C) = P(B|AC)P(A|C) = P(B|C)P(A|C)$

Example

- 60% of ML students pass the final and 45% of ML students pass both the final and the midterm *
- What percent of students who passed the final also passed the midterm?

* These are made up values.

Example

- 60% of ML students pass the final and 45% of ML students pass both the final and the midterm *
- What percent of students who passed the final also passed the midterm?

- Reworded: What percent of students passed the midterm given they passed the final?
- $P(M|F) = P(M,F) / P(F)$
- $= .45 / .60$
- $= .75$

* These are made up values.

Marginalization and Law of Total Probability

- Marginalization (Sum Rule)

$$p(x) = \sum_y p(x, y)$$

I should make example of both!!!!!!! Maybe even visualization of sum rule, some over matrix of probs

- Law of Total Probability

$$p(x) = \sum_y p(x \mid y) \cdot p(y)$$

Bayes' Rule

P(A|B) = P(AB) /P(B) (Conditional Probability)

P(A|B) = P(B|A)P(A) /P(B) (Product Rule)

P(A|B) = P(B|A)P(A) / Σ P(B|A)P(A) (Law of Total Probability)

$$P(A|B) = \frac{P(A)\,P(B|A)}{P(B)}$$

$$P(B) = \sum_j P(B \mid A_j)P(A_j)$$

Bayes' Rule

$$P(A|B) = \frac{P(A)\,P(B|A)}{P(B)}$$

$$p(\theta|x) = \frac{p(x|\theta)p(\theta)}{p(x)}.$$

$$\text{Posterior} = \frac{\text{Likelihood} * \text{Prior}}{\text{Evidence}}$$

$$\text{Posterior probability} \propto \text{Likelihood} \times \text{Prior probability}$$

Example

- Suppose you have tested positive for a disease; what is the probability that you actually have the disease?
- It depends on the accuracy and sensitivity of the test, and on the background (prior) probability of the disease.
- $P(T=1|D=1) = .95$ (true positive)
- $P(T=1|D=0) = .10$ (false positive)
- $P(D=1) = .01$ (prior)

- $P(D=1|T=1) = ?$

Example

- $P(T=1|D=1) = .95$ (true positive)
- $P(T=1|D=0) = .10$ (false positive)
- $P(D=1) = .01$ (prior)

Bayes' Rule

- $P(D|T) = P(T|D)P(D) / P(T)$

$= .95 * .01 / .1085$

$= .087$

Law of Total Probability

- $P(T) = \Sigma\, P(T|D)P(D)$

$= P(T|D=1)P(D=1) + P(T|D=0)P(D=0)$

$= .95*.01 + .1*.99$

$= .1085$

The probability that you have the disease given you tested positive is 8.7%

Random Variable

- How do we link sample spaces and events to data?
- A random variable is a mapping that assigns a real number $X(\omega)$ to each outcome ω

- Example: Flip a coin ten times. Let $X(\omega)$ be the number of heads in the sequence ω. If ω = HHTHHTHHTT, then $X(\omega) = 6$.

Discrete vs Continuous Random Variables

- Discrete: can only take a countable number of values
- Example: number of heads
- Distribution defined by probability mass function (pmf)
- Marginalization: $$p(x) = \sum_y p(x, y)$$

- Continuous: can take infinitely many values (real numbers)
- Example: time taken to accomplish task
- Distribution defined by probability density function (pdf)
- Marginalization: $$p(x) = \int_y p(x, y)\, dy$$

Probability Distribution Statistics

- Mean: E[x] = μ = first moment $= \int_{-\infty}^{\infty} x f(x)\,\mathrm{d}x$ Univariate continuous random variable

  $= \sum_{i=1}^{\infty} x_i\, p_i$ Univariate discrete random variable

- Variance: Var(X) = $\operatorname{E}\left[(X-\mu)^2\right] = \int (x-\mu)^2 f(x)\,dx$

$$
\begin{aligned}
&= \operatorname{E}\left[(X-\operatorname{E}[X])^2\right] \\
&= \operatorname{E}\left[X^2 - 2X\operatorname{E}[X] + (\operatorname{E}[X])^2\right] \\
&= \operatorname{E}\left[X^2\right] - 2\operatorname{E}[X]\operatorname{E}[X] + (\operatorname{E}[X])^2 \\
&= \operatorname{E}\left[X^2\right] - (\operatorname{E}[X])^2
\end{aligned}
$$

- Nth moment = $\int_{-\infty}^{\infty} (x-c)^n\, f(x)\,dx$

Bernoulli Distribution

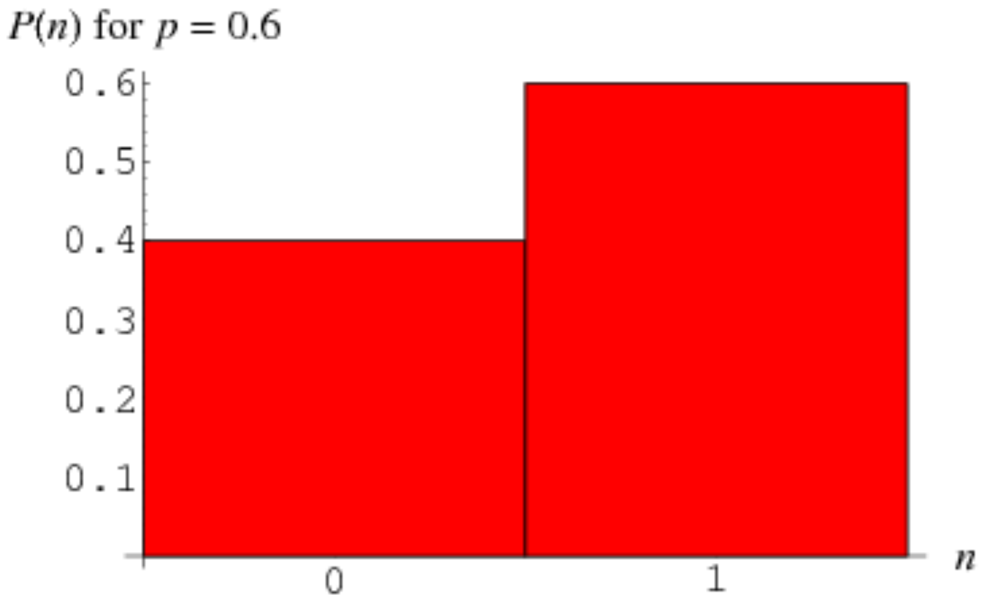
- RV: x $\in$ {0, 1}
- Parameter: μ

$$\mathrm{Bern}(x|\mu) = \mu^x(1-\mu)^{1-x}$$

- Mean = E[x] = μ
- Variance = $\mu(1-\mu)$

Example: Probability of flipping heads (x=1) with a unfair coin

$$= .6^1\ (1-.6)^{1-1}$$
$$= \ .6$$



Binomial Distribution

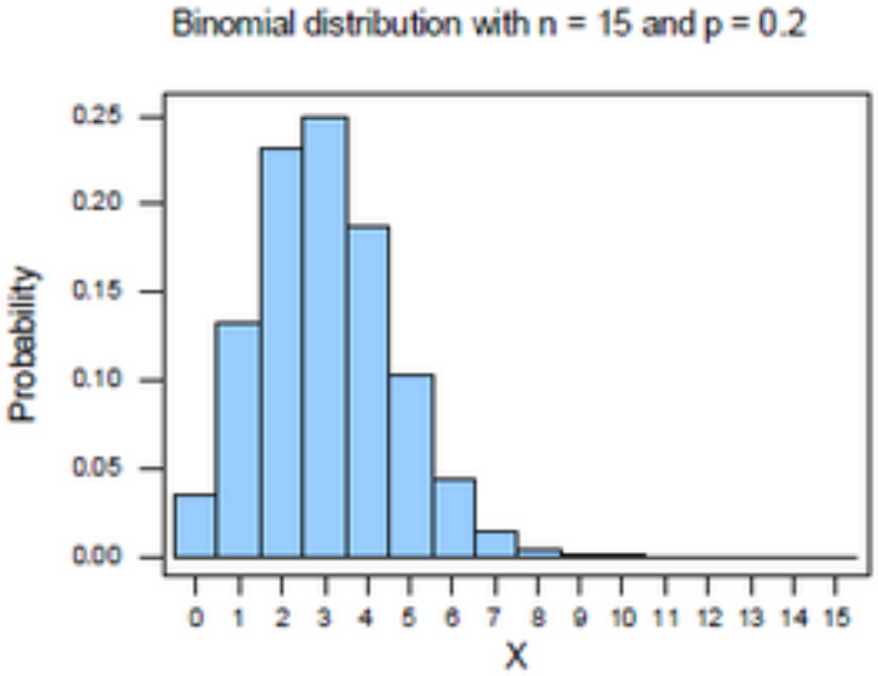
- RV: m = number of successes
- Parameters: N = number of trials

  μ = probability of success

$$\mathrm{Bin}(m|N,\mu) = \binom{N}{m}\mu^m(1-\mu)^{N-m}$$

- Mean = E[x] = Nμ
- Variance = N$\mu(1-\mu)$

Example: Probability of flipping heads m times out of 15 independent flips with success probability 0.2



Multinomial Distribution

- The multinomial distribution is a generalization of the binomial distribution to k categories instead of just binary (success/fail)
- For **n independent trials** each of which leads to a **success for exactly one of k categories**, the multinomial distribution gives the probability of any particular combination of numbers of successes for the various categories
- Example: Rolling a die N times

Multinomial Distribution

- RVs: $m_1 \ldots m_K$ (counts)
- Parameters: N = number of trials

  $\boldsymbol{\mu} = \mu_1 \ldots \mu_K$ probability of success for each category, $\Sigma\boldsymbol{\mu}=1$

$$\mathrm{Mult}(m_1, m_2, \ldots, m_K|\boldsymbol{\mu}, N) = \binom{N}{m_1 m_2 \ldots m_K} \prod_{k=1}^{K} \mu_k^{m_k}$$

- Mean of m_k: $N\mu_k$
- Variance of m_k: $N\mu_k(1-\mu_k)$

Multinomial Distribution

Ex: Rolling 2 on a fair die 5 times out of 10 rolls.

- RVs: $m_1 \dots m_K$ (counts) → [0, 5, 0, 0, 0, 0]
- Parameters: N = number of trials → 10

  $\boldsymbol{\mu} = \mu_1 \dots \mu_K$ probability of success for each category, $\Sigma\boldsymbol{\mu}=1$

  [1/6, 1/6, 1/6, 1/6, 1/6, 1/6]

$$\mathrm{Mult}(m_1, m_2, \dots, m_K|\boldsymbol{\mu}, N) = \binom{N}{m_1 m_2 \dots m_K} \prod_{k=1}^{K} \mu_k^{m_k}$$

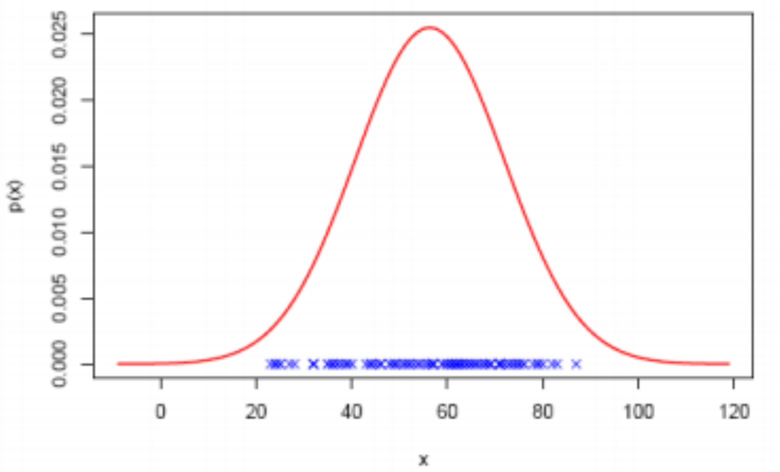
- Mean of m_k: $N\mu_k$
- Variance of m_k: $N\mu_k(1-\mu_k)$

$$\binom{10}{5}\frac{1}{6}^5 = \frac{7}{216}$$

Gaussian Distribution

- Aka the normal distribution
- Widely used model for the distribution of continuous variables
- In the case of a single variable x, the Gaussian distribution can be written in the form

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



- where μ is the mean and σ^2 is the variance

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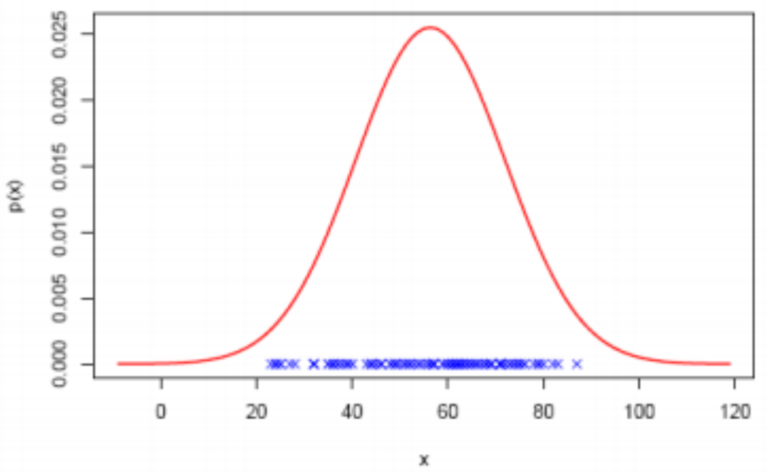
normalization constant

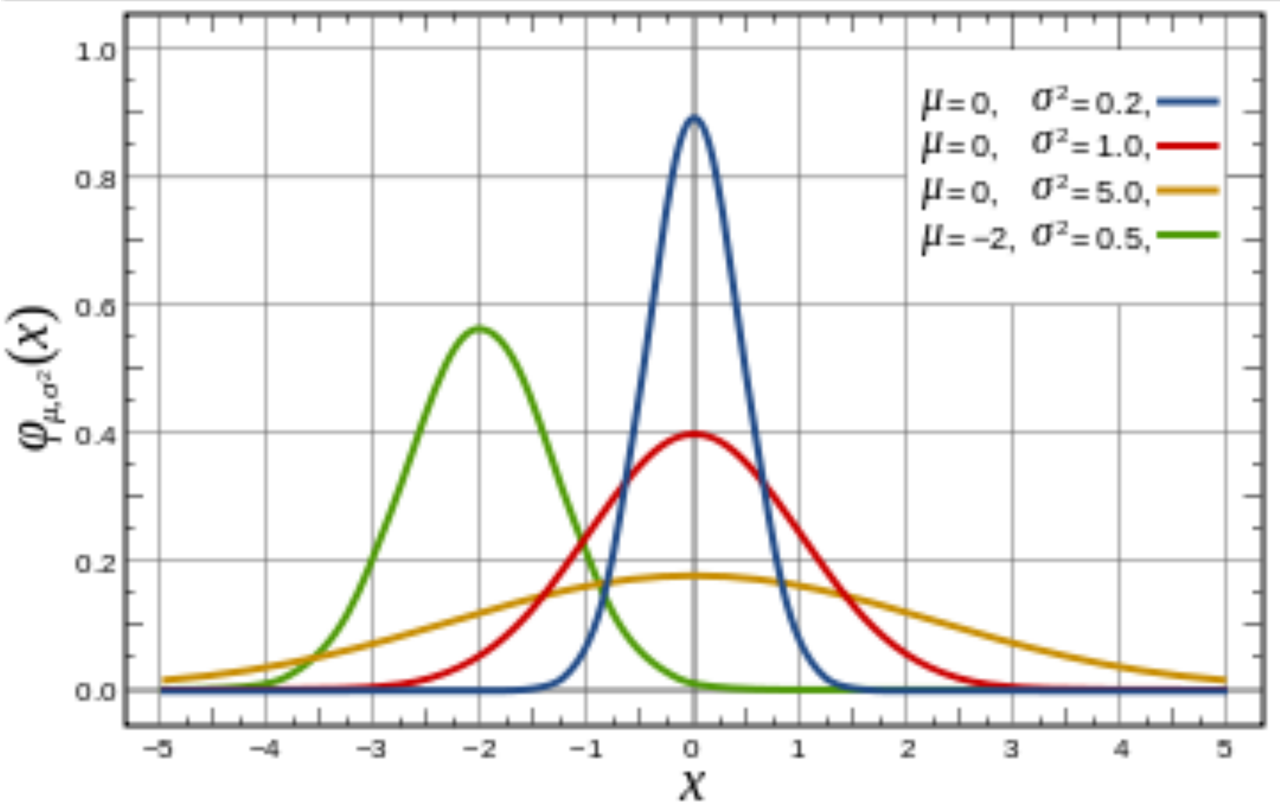
$e^{(-squared\ distance\ from\ mean)}$



- where μ is the mean and σ^2 is the variance

Gaussian Distribution

- Gaussians with different means and variances

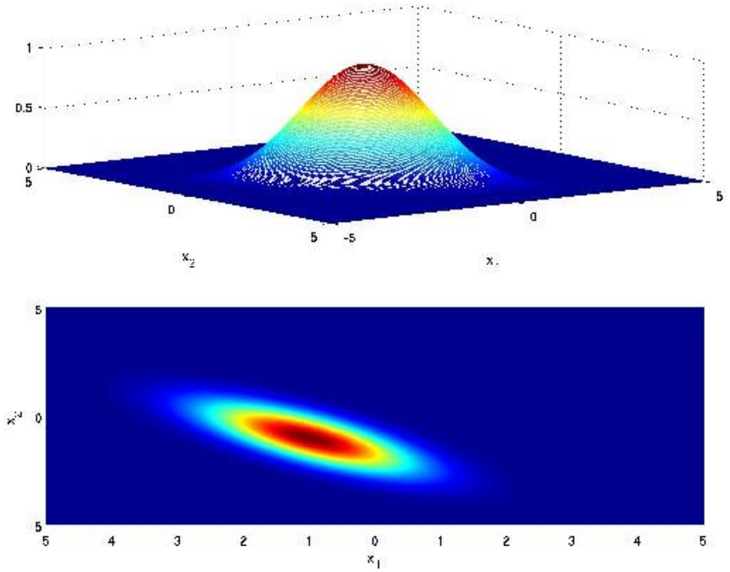


Multivariate Gaussian Distribution

- For a D-dimensional vector **x**, the multivariate Gaussian distribution takes the form

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

- where μ is a D-dimensional mean vector
- Σ is a D × D covariance matrix
- |Σ| denotes the determinant of Σ



Inferring Parameters

- We have data X and we assume it comes from some distribution
- How do we figure out the parameters that 'best' fit that distribution?
  - Maximum Likelihood Estimation (MLE)

$$\tilde{\pi}_{MLE} = \underset{\pi}{\operatorname{argmax}}\, P(\mathcal{X}|\pi)$$

  - Maximum a Posteriori (MAP)

$$\tilde{\pi}_{MAP} = \underset{\pi}{\operatorname{argmax}}\, P(\pi|\mathcal{X})$$

See 'Gibbs Sampling for the Uninitiated' for a straightforward introduction to parameter estimation: http://www.umiacs.umd.edu/~resnik/pubs/LAMP-TR-153.pdf

I.I.D.

- Random variables are independent and identically distributed (i.i.d.) if they have the same probability distribution as the others and are all mutually independent.

- Example: Coin flips are assumed to be IID

MLE for parameter estimation

- The parameters of a Gaussian distribution are the mean (μ) and variance (σ^2)

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

- We'll estimate the parameters using MLE
- Given observations $x_1, \ldots, x_N$, the likelihood of those observations for a certain μ and σ^2 (assuming IID) is

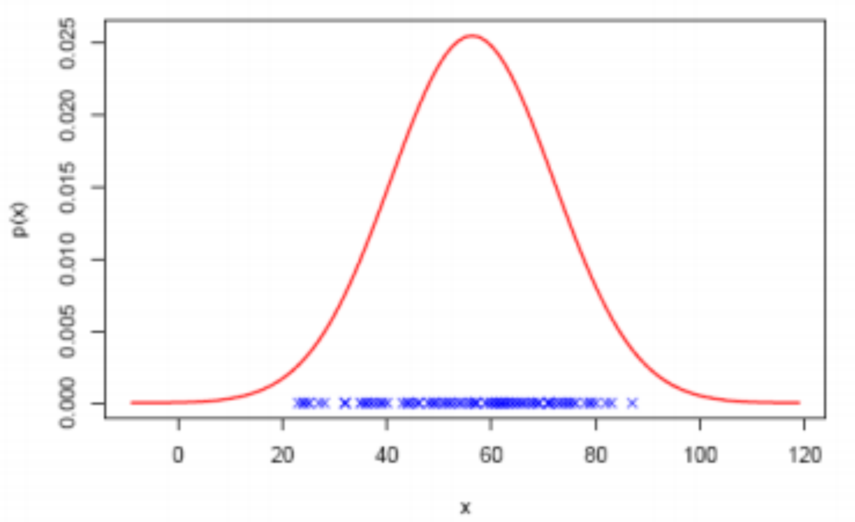
Likelihood = $$p(x_1,\ldots,x_N|\mu,\sigma^2) = \prod_{n=1}^{N} \frac{1}{\sqrt{2\pi}\sigma} \exp\left\{\frac{-(x_n-\mu)^2}{2\sigma^2}\right\}$$

Recall: If IID, P(ABC) = P(A)P(B)P(A)

MLE for parameter estimation

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

Likelihood = $p(x_1,\ldots,x_N|\mu,\sigma^2) = \prod_{n=1}^{N} \frac{1}{\sqrt{2\pi}\sigma} \exp\left\{\frac{-(x_n-\mu)^2}{2\sigma^2}\right\}$



What's the distribution's mean and variance?

MLE for Gaussian Parameters

Likelihood = $p(x_1, \ldots, x_N|\mu, \sigma^2) = \prod_{n=1}^{N} \frac{1}{\sqrt{2\pi}\sigma} \exp\left\{\frac{-(x_n - \mu)^2}{2\sigma^2}\right\}$

- Now we want to maximize this function wrt μ
- Instead of maximizing the product, we take the log of the likelihood so the product becomes a sum

Log Likelihood = log $p(x_1, \ldots, x_N|\mu, \sigma^2) = \sum_{n=1}^{N}$ Log $\frac{1}{\sqrt{2\pi}\sigma} \exp\left\{\frac{-(x_n - \mu)^2}{2\sigma^2}\right\}$

- We can do this because log is monotonically increasing
- Meaning

$$\max L(\theta) = \max \log L(\theta)$$

MLE for Gaussian Parameters

- Log Likelihood simplifies to:

$$\mathcal{L}(\mu, \sigma) = -\frac{1}{2} N \log(2\pi\sigma^2) - \sum_{n=1}^{N} \frac{(x_n - \mu)^2}{2\sigma^2}$$

- Now we want to maximize this function wrt μ
- How?

To see proofs for these derivations: http://www.statlect.com/normal_distribution_maximum_likelihood.htm

MLE for Gaussian Parameters

- Log Likelihood simplifies to:

$$\mathcal{L}(\mu, \sigma) = -\frac{1}{2} N \log(2\pi\sigma^2) - \sum_{n=1}^{N} \frac{(x_n - \mu)^2}{2\sigma^2}$$

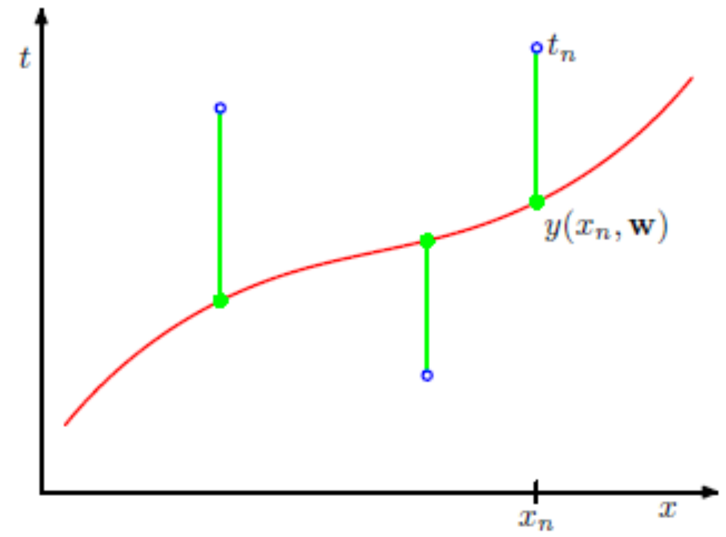
- Now we want to maximize this function wrt μ
- Take the derivative, set to 0, solve for μ

$$\hat{\mu} = \frac{1}{N} \sum_{n=1}^{N} x_n \qquad \hat{\sigma^2} = \frac{1}{N} \sum_{n=1}^{N} (x_n - \hat{\mu})^2$$

To see proofs for these derivations: http://www.statlect.com/normal_distribution_maximum_likelihood.htm

Maximum Likelihood and Least Squares

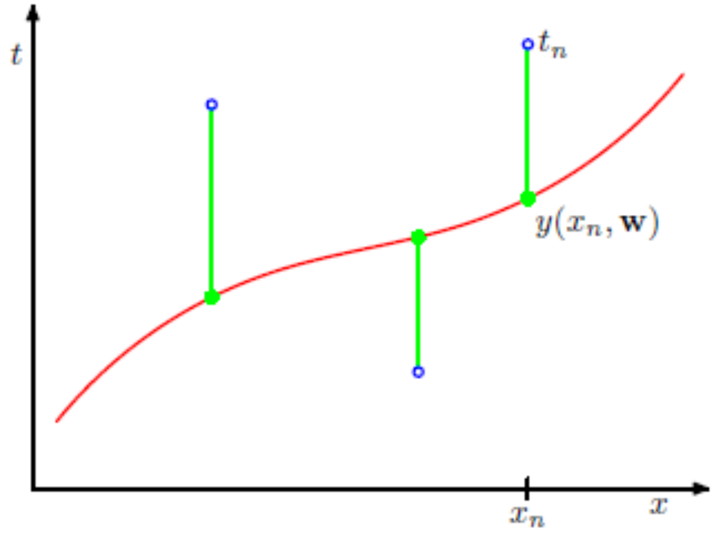
- Suppose that you are presented with a sequence of data points $(X_1, T_1), \ldots, (X_n, T_n)$, and you are asked to find the "best fit" line passing through those points.
- In order to answer this you need to know precisely how to tell whether one line is "fitter" than another
- A common measure of fitness is the squared-error $$\sum_{n=1}^{N}[t^{(n)} - y^{(n)}]^2$$



For a good discussion of Maximum likelihood estimators and least squares see http://people.math.gatech.edu/~ecroot/3225/maximum_likelihood.pdf

Maximum Likelihood and Least Squares

y(x,w) is estimating the target t



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

- Error/Loss/Cost/Objective function measures the squared error

Green lines $$\ell(\mathbf{w}) = \sum_{n=1}^{N} [t^{(n)} - y^{(n)}]^2$$

- Least Square Regression
  - Minimize L(w) wrt w

Maximum Likelihood and Least Squares

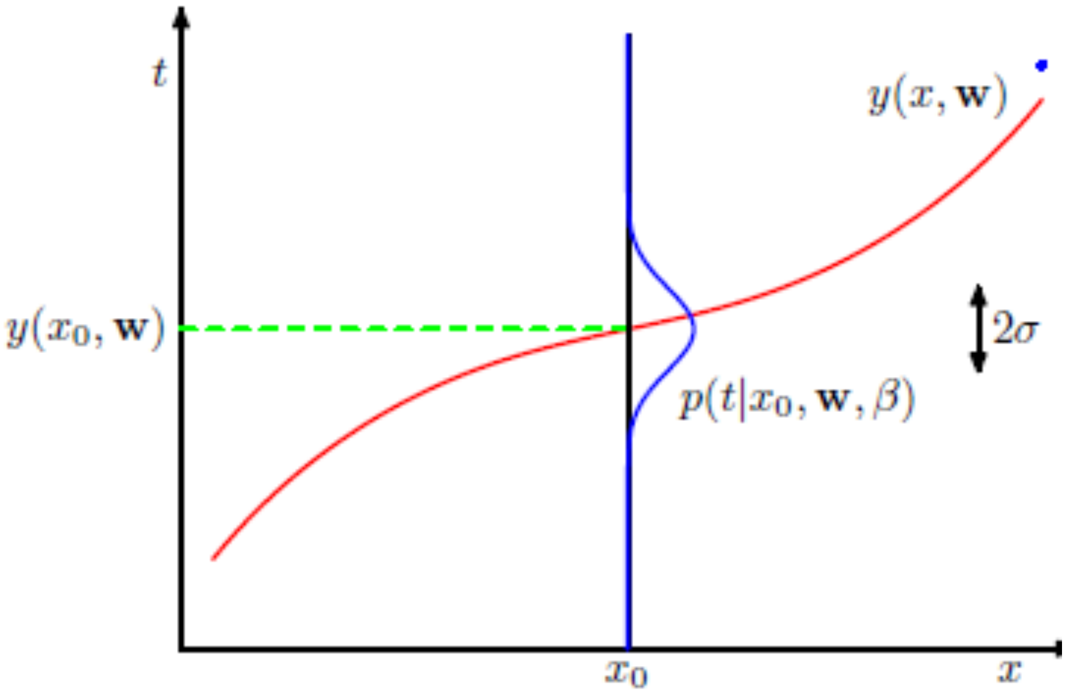
- Now we approach curve fitting from a probabilistic perspective
- We can express our uncertainty over the value of the target variable using a probability distribution
- We assume, given the value of x, the corresponding value of t has a Gaussian distribution with a mean equal to the value y(x,w)

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

β is the precision parameter (inverse variance)

Maximum Likelihood and Least Squares

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



Maximum Likelihood and Least Squares

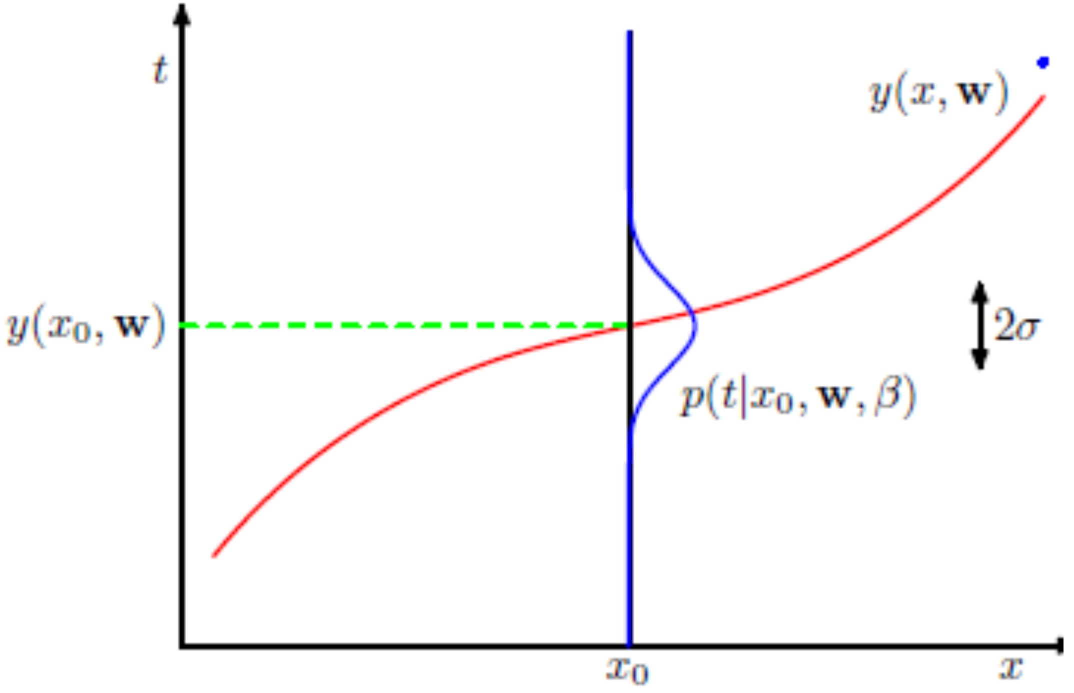
- We now use the training data {x, t} to determine the values of the unknown parameters w and β by maximum likelihood

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

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

- Log Likelihood

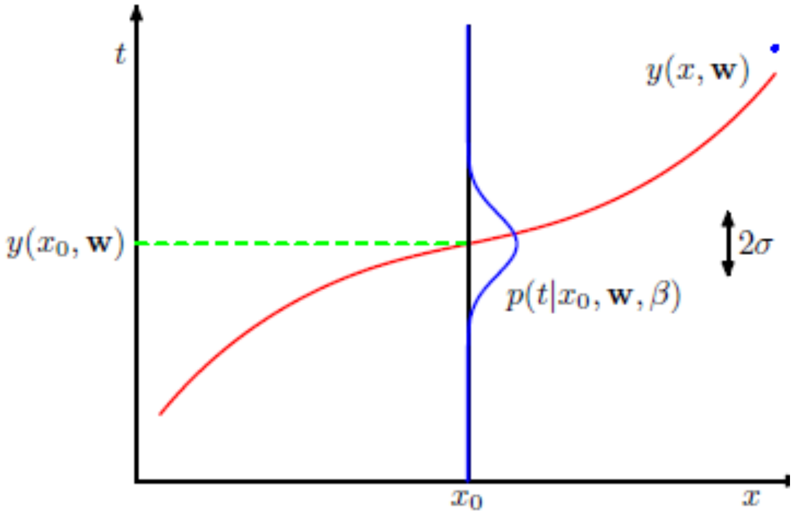
$$\ln p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta) = -\frac{\beta}{2}\sum_{n=1}^{N}\{y(x_n, \mathbf{w}) - t_n\}^2 + \frac{N}{2}\ln\beta - \frac{N}{2}\ln(2\pi)$$



Maximum Likelihood and Least Squares

- Log Likelihood

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



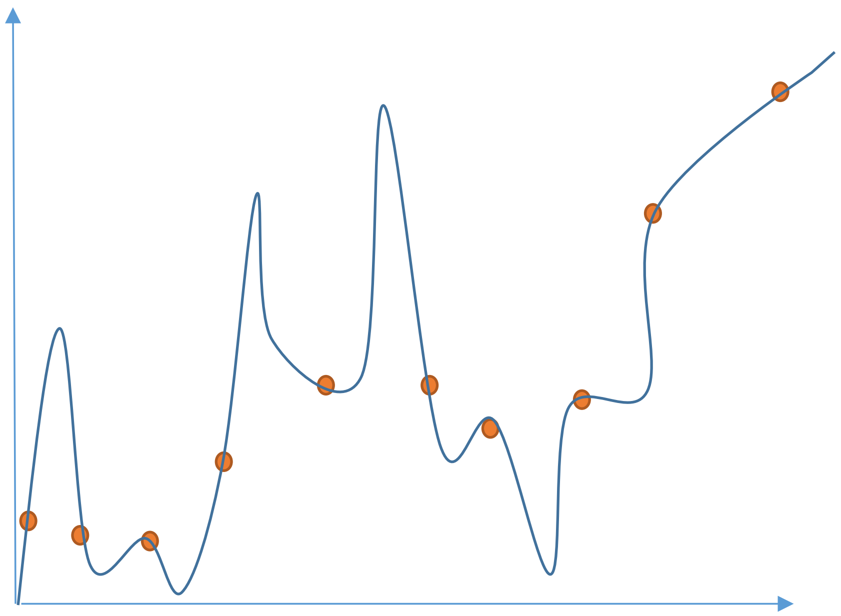
- Maximize Log Likelihood wrt to w
- Since last two terms, don't depend on w, they can be omitted.
- Also, scaling the log likelihood by a positive constant β/2 does not alter the location of the maximum with respect to w, so it can be ignored
- Result: Maximize $-\sum_{n=1}^{N}\{y(x_n, \mathbf{w}) - t_n\}^2$

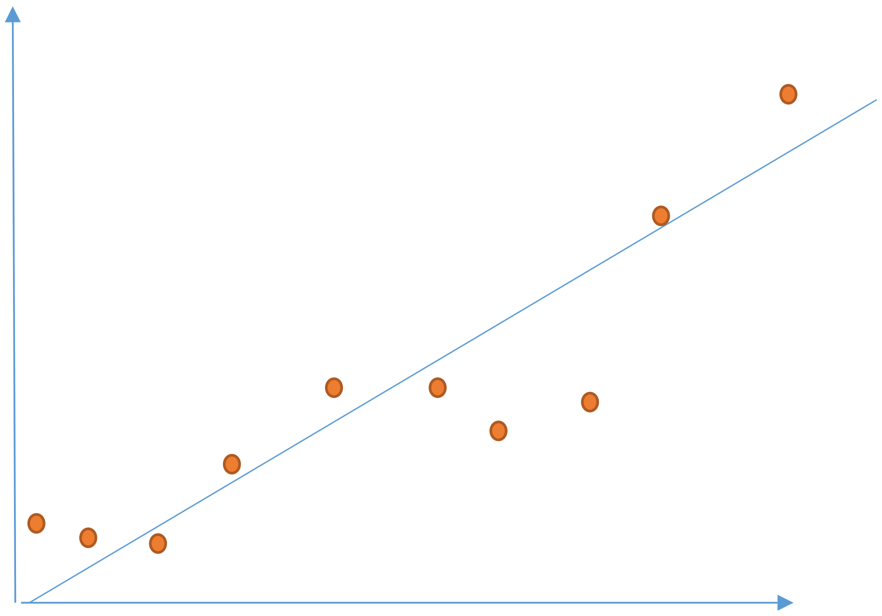
Maximum Likelihood and Least Squares

- MLE
  - Maximize $-\sum_{n=1}^{N}\{y(x_n,\mathbf{w})-t_n\}^2$
- Least Squares
  - Minimize $\sum_{n=1}^{N}[t^{(n)}-y^{(n)}]^2$
- Therefore, maximizing likelihood is equivalent, so far as determining w is concerned, to minimizing the sum-of-squares error function
- Significance: sum-of-squares error function arises as a consequence of maximizing likelihood under the assumption of a Gaussian noise distribution

Matlab Linear Regression Demo

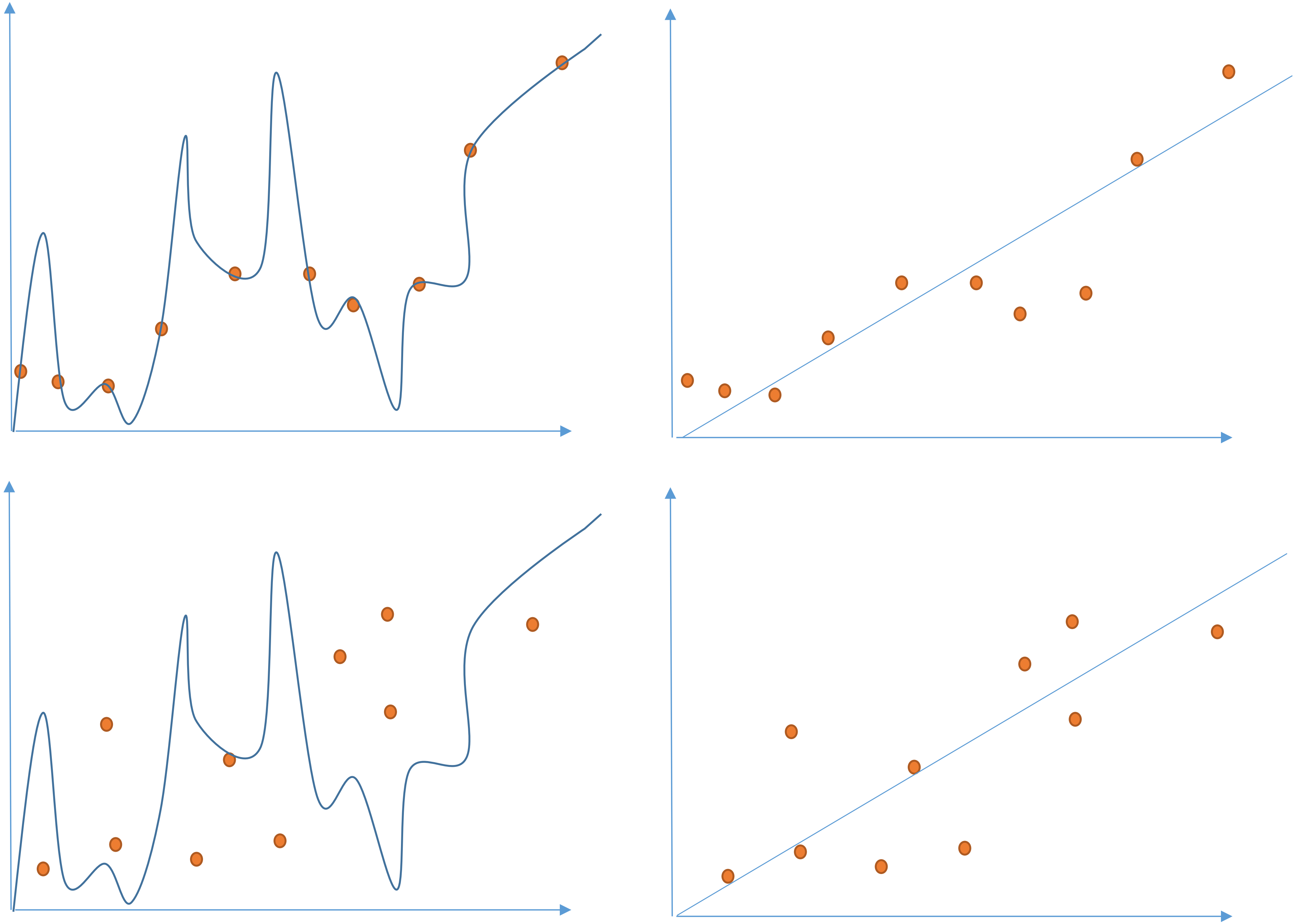
Training Set



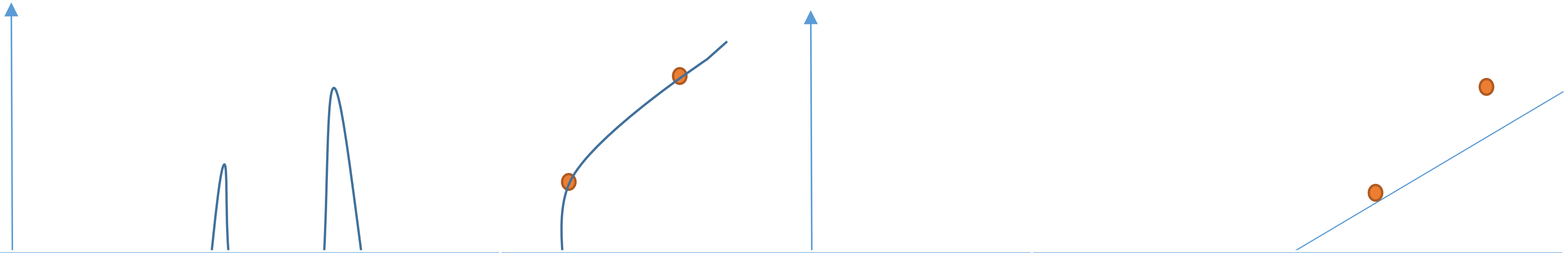


Training Set

Validation Set
Held Out Data

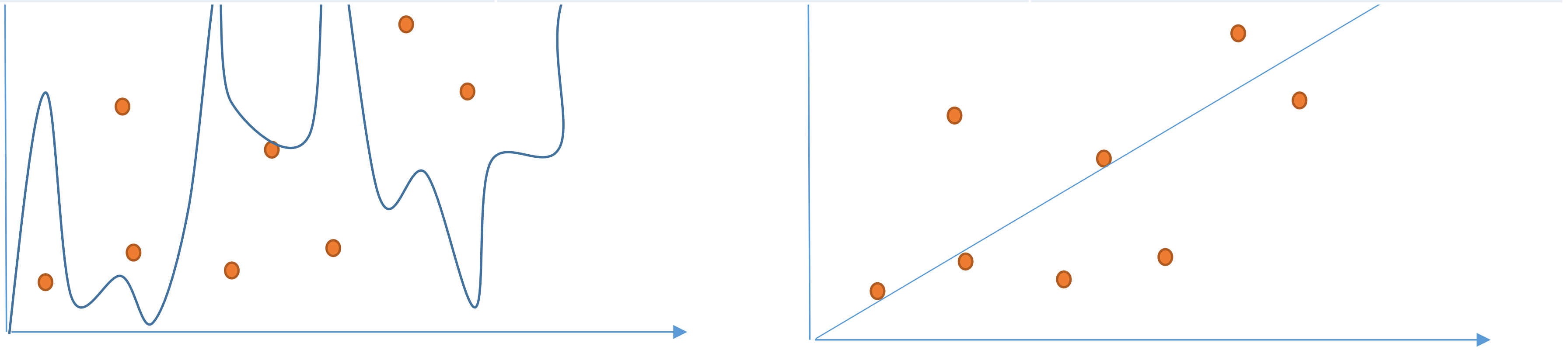


Training Set



	Training Set Error	Validation Set Error
Linear	++++	+++++
Quadratic	+++	++++++
Cubic	++	+++++++
4^{th} degree polynomial	+	++++++++

Validation Set
Held Out Data



	Training Set Error	Validation Set Error
Linear	++++	+++++
Quadratic	+++	++++++
Cubic	++	+++++++
4^{th} degree polynomial	+	++++++++

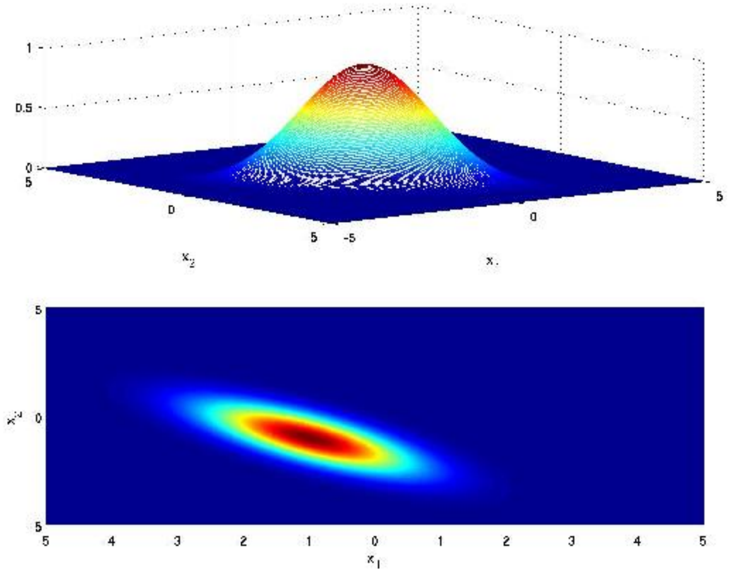
How well your model generalizes to new data is what matters!

Multivariate Gaussian Distribution

- For a D-dimensional vector **x**, the multivariate Gaussian distribution takes the form

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

- where μ is a D-dimensional mean vector
- Σ is a D × D covariance matrix
- |Σ| denotes the determinant of Σ



Covariance Matrix

$$Cov(X,Y) = \int_{S_2}\int_{S_1}(x-\mu_X)(y-\mu_Y)f(x,y)dxdy$$

$$\Sigma_{ij} = \mathrm{cov}(X_i, X_j) = \mathrm{E}\left[(X_i-\mu_i)(X_j-\mu_j)\right]$$

$$\Sigma = \begin{bmatrix} \mathrm{E}[(X_1-\mu_1)(X_1-\mu_1)] & \mathrm{E}[(X_1-\mu_1)(X_2-\mu_2)] & \cdots & \mathrm{E}[(X_1-\mu_1)(X_n-\mu_n)] \\ \mathrm{E}[(X_2-\mu_2)(X_1-\mu_1)] & \mathrm{E}[(X_2-\mu_2)(X_2-\mu_2)] & \cdots & \mathrm{E}[(X_2-\mu_2)(X_n-\mu_n)] \\ \vdots & \vdots & \ddots & \vdots \\ \mathrm{E}[(X_n-\mu_n)(X_1-\mu_1)] & \mathrm{E}[(X_n-\mu_n)(X_2-\mu_2)] & \cdots & \mathrm{E}[(X_n-\mu_n)(X_n-\mu_n)] \end{bmatrix}$$

Questions?