https://uva-iai.github.io

Apply for the Inclusive AI Mentorship program

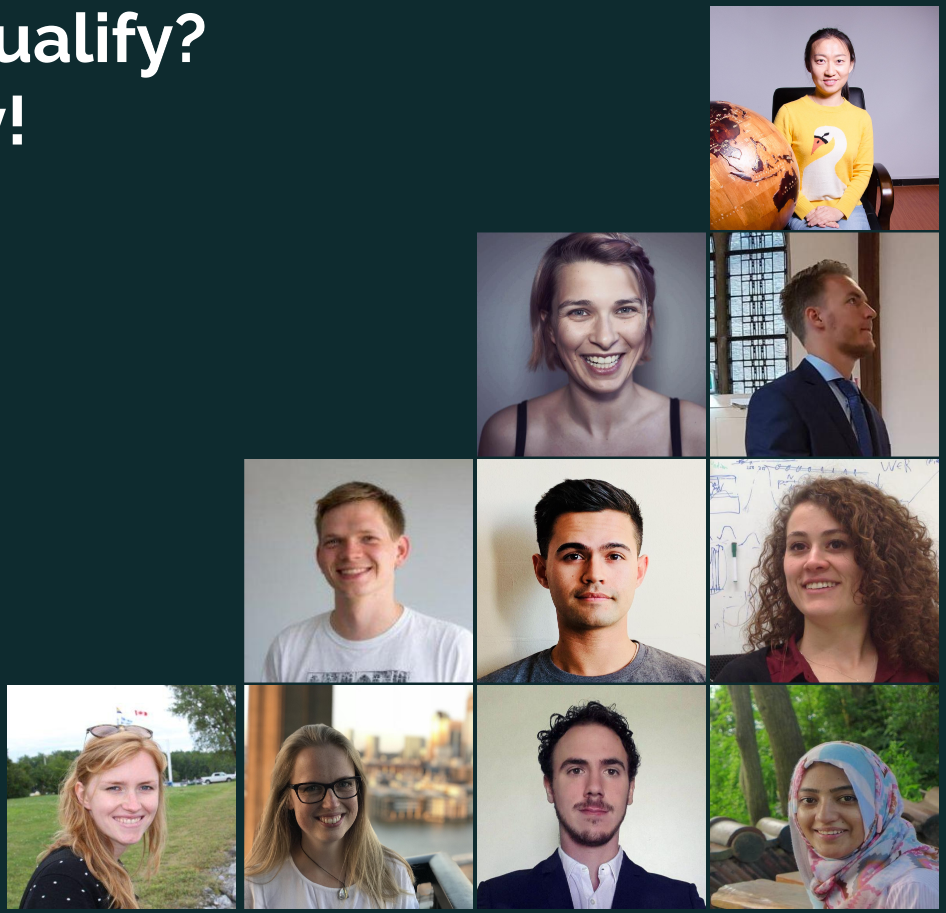
Unique opportunity to get advice from senior peers (PhDs, postdocs and assistant profs) from academia and industry!

For underrepresented groups

Unsure if you qualify? Apply anyway!

Mentees should expect to be able to:

- ask mentor for practical advice, e.g. how to write a CV or motivation letter, where to apply for jobs, when to apply for PhDs
- network with other students
- seek non-academic advice from mentor
- learn how to present their research
- connect with other researchers



Machine Learning 1

- Lecture 2 -

Supervised Learning: Linear Regression

-Patrick Forré-

Slides created by:
Rianne van den Berg

Image credit: Kirillm | Getty Images

Discussion forum

Piazza:

piazza.com/university_of_amsterdam/fall2019/ml1

If you have not found a lab partner, use Piazza to find one!

Overview

1. **Probability theory**

2. **Statistical learning principles:**

    I. Maximum likelihood

    II. Maximum a posteriori

    III. Bayesian prediction

Overview

1. **Probability theory**

2. Statistical learning principles**:**

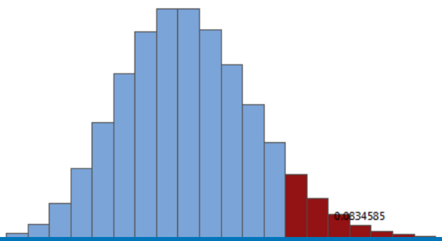
   I. Maximum likelihood

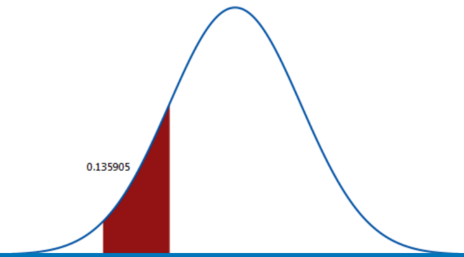
   II. Maximum a posteriori

   III. Bayesian prediction

The rules of probability theory

For random variables *X* ∊ $\mathcal{X}$ and *Y* ∊ $\mathcal{Y}$:





	Discrete	Continous
Additivity	$p(X \in A) = \sum_{x \in A} p(x)$	
Positivity	$p(x) \geq 0$	$p(x) \geq 0$
Normalization		$\int_{\mathcal{X}} p(x) dx = 1$
Sum Rule	$p(x) = \sum_{y \in \mathcal{Y}} p(x, y)$	
Product Rule	$p(x, y) = p(x \mid y) p(y)$	$p(x, y) = p(x \mid y) p(y)$

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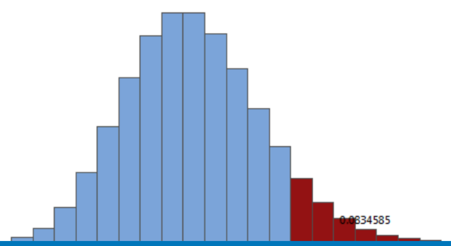

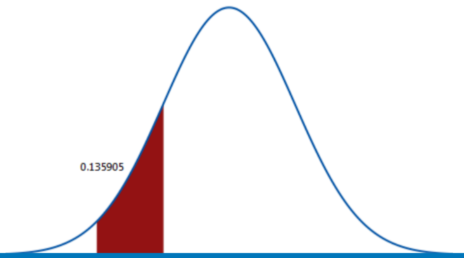

	Discrete	Continous
Additivity	$p(X \in A) = \sum_{x \in A} p(x)$	$p(X \in A) = \int_A p(x)$
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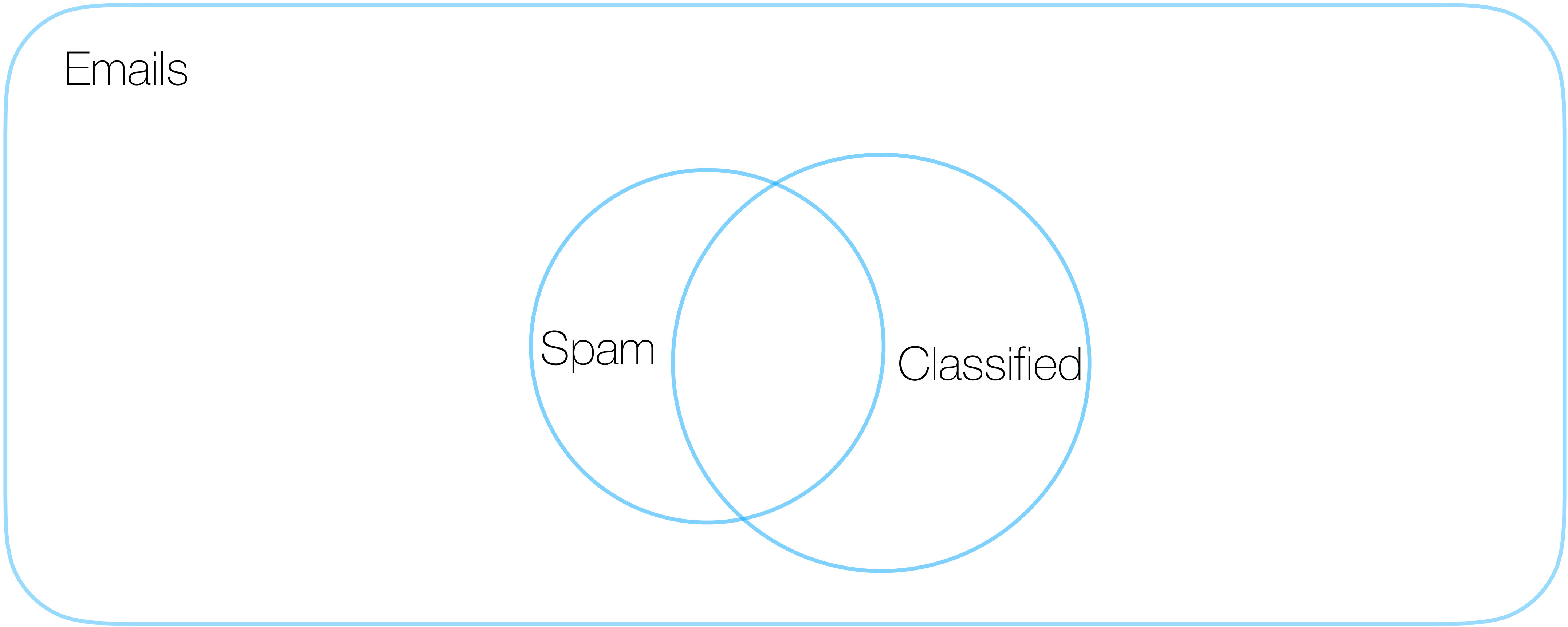
Product Rule	$p(x, y) = p(x\|y)p(y)$	$p(x, y) = p(x\|y)p(y)$

Bayes Rule

$$p(y|x) = \frac{p(x|y)p(y)}{p(x)}$$

- *p(y)* : the prior probability of *Y* = *y*
- *p(y | x)* : the posterior probability of *Y* = *y*
- *p(x | y)* : the likelihood of *X* = *x* given *Y* = *y*
- *p(x)* : the evidence for X = x

Bayes Rule



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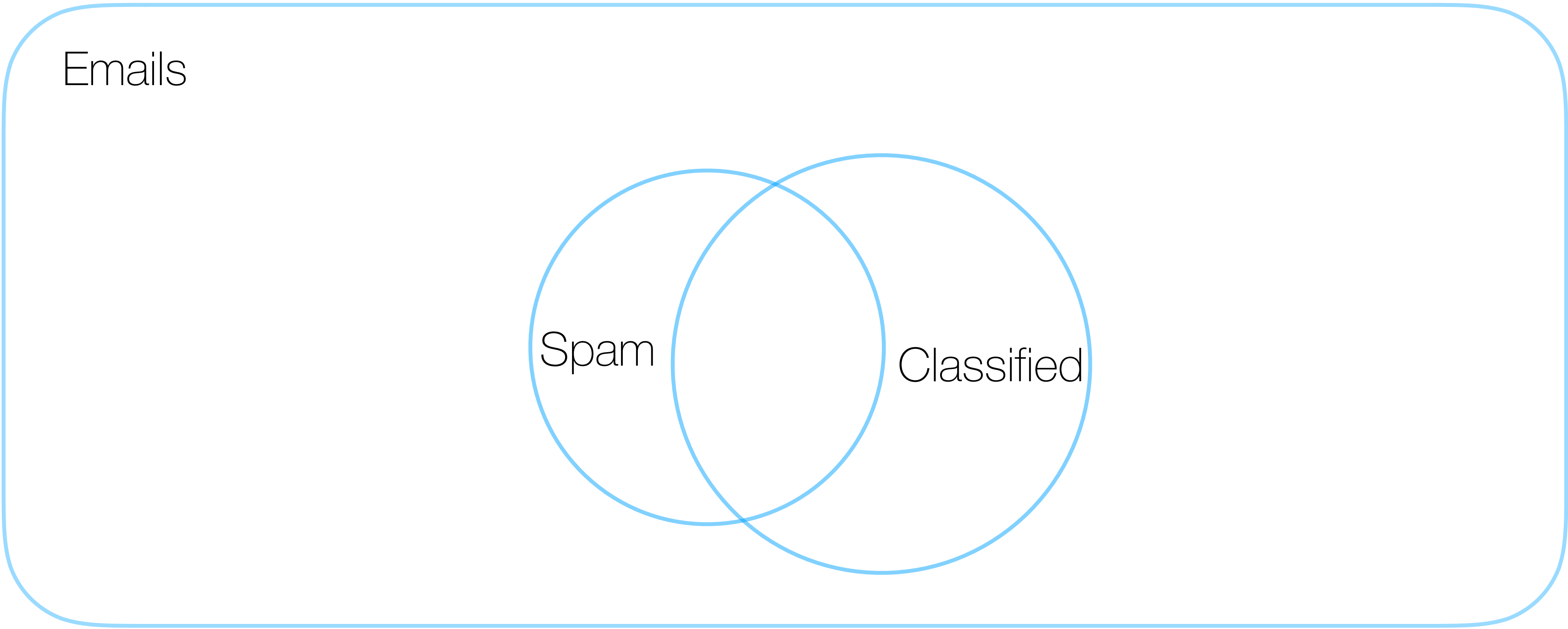
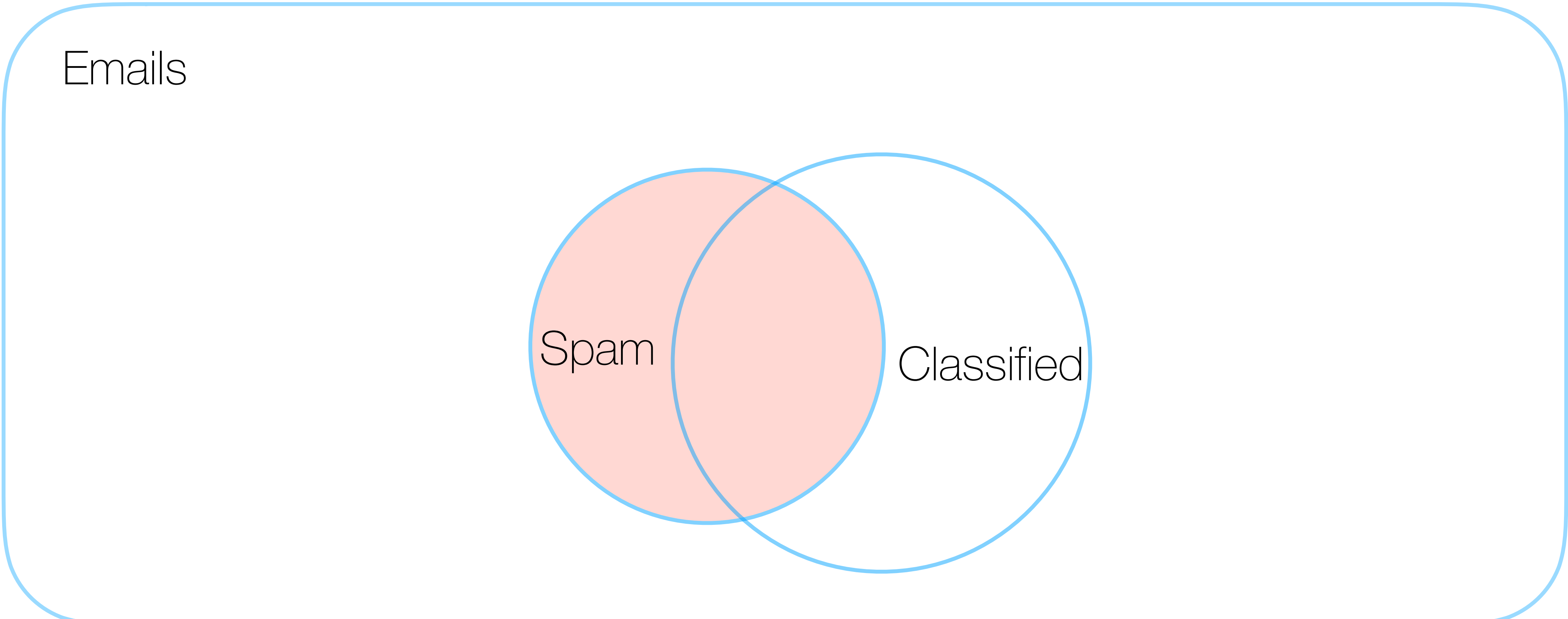


$$p(S) = \frac{S}{E}$$

Bayes Rule



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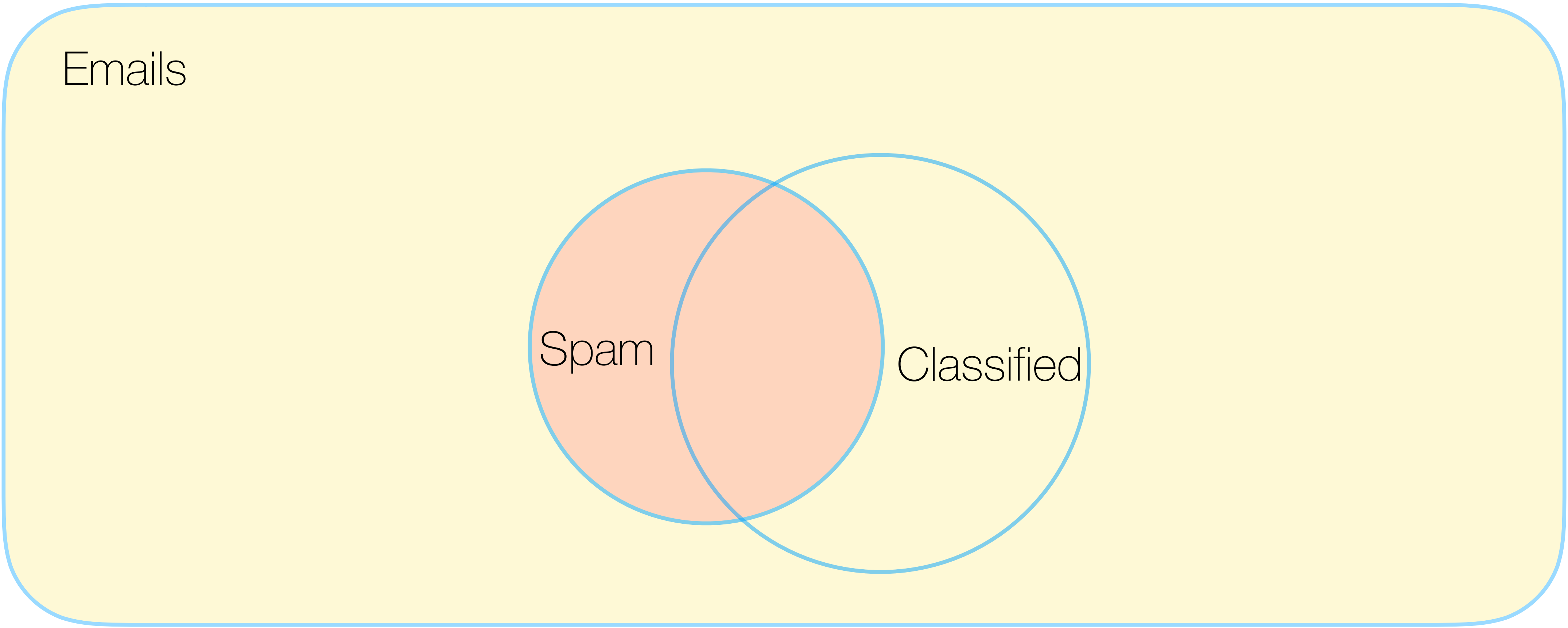

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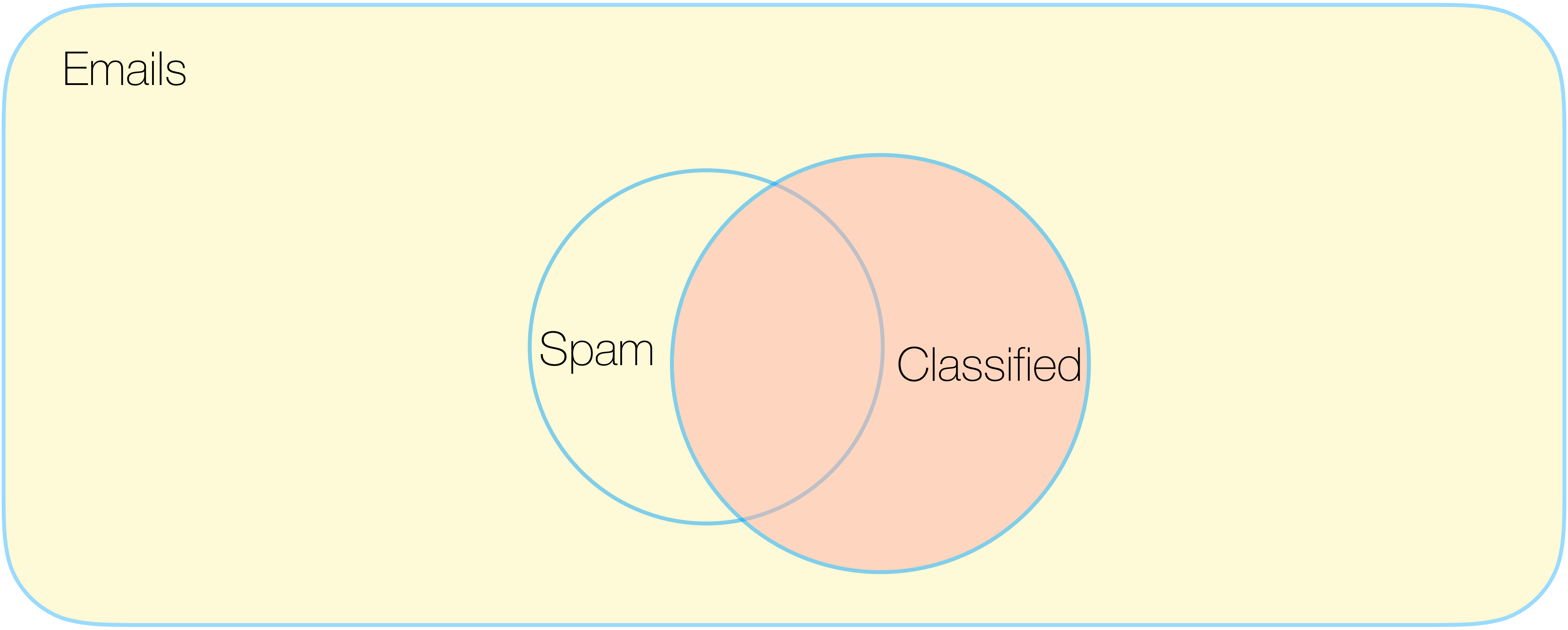
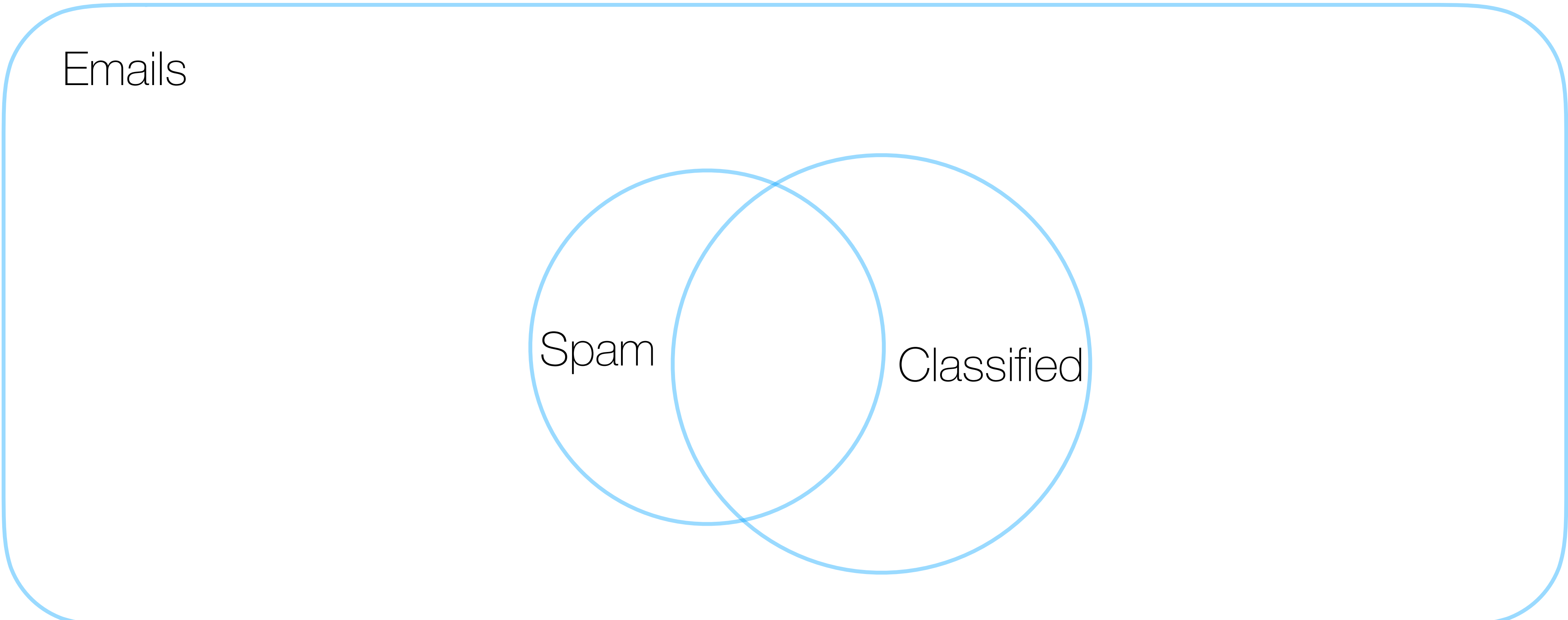


$$p(S) = \frac{S}{E}$$

$$p(C) = \frac{C}{E}$$

Bayes Rule



$$p(S) = \frac{S}{E}$$

$$p(S|C) = \frac{S \cap C}{C}$$

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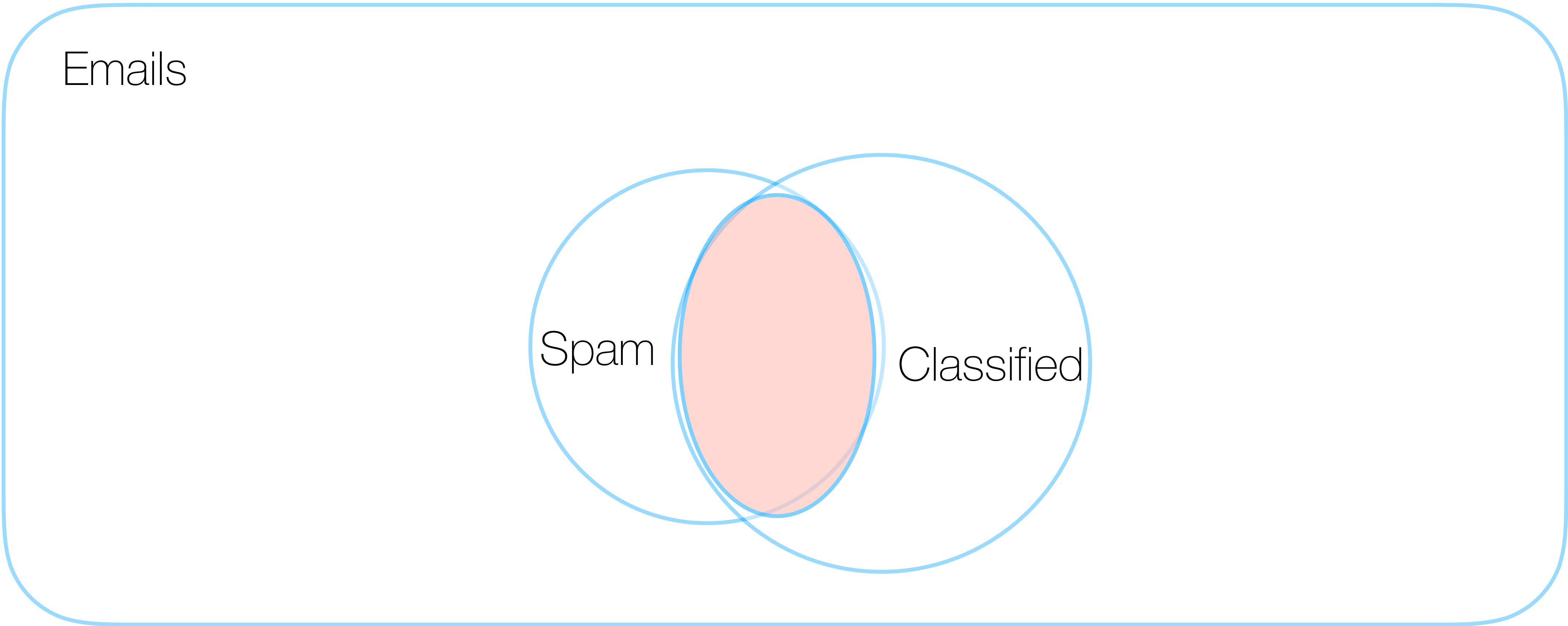

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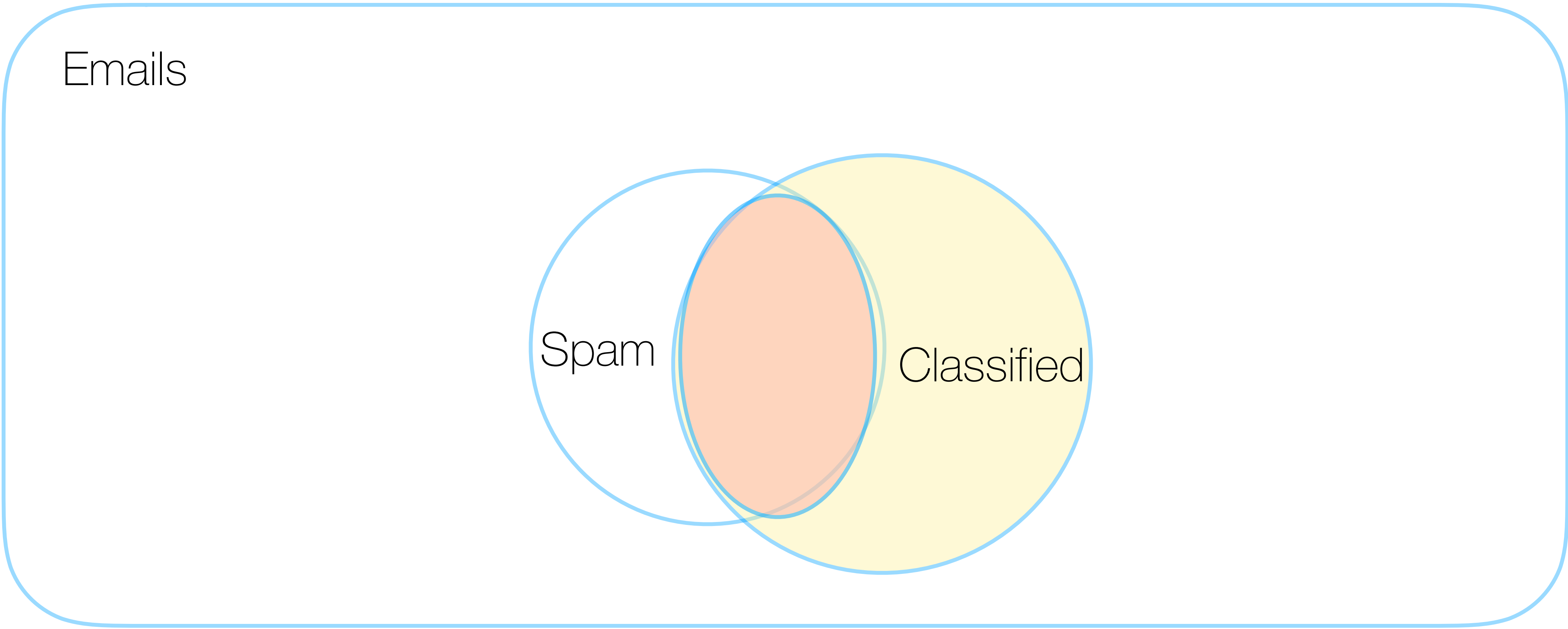

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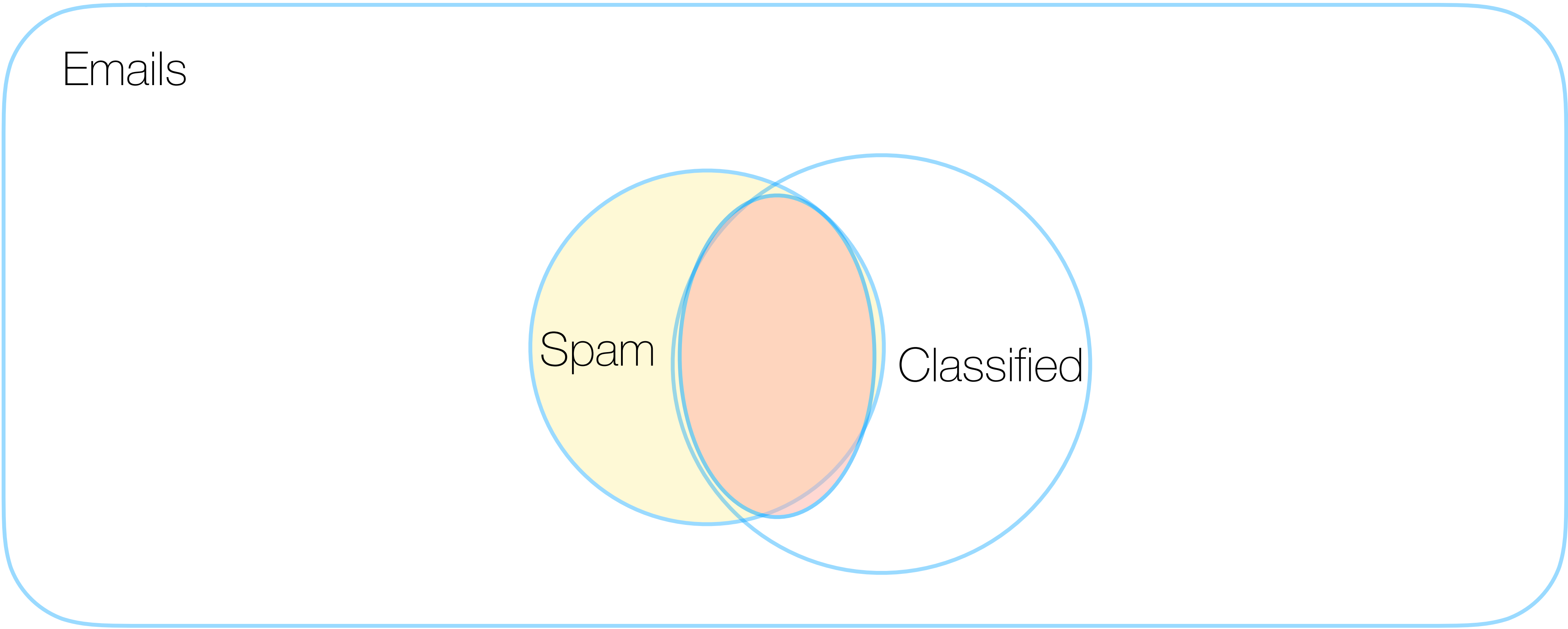

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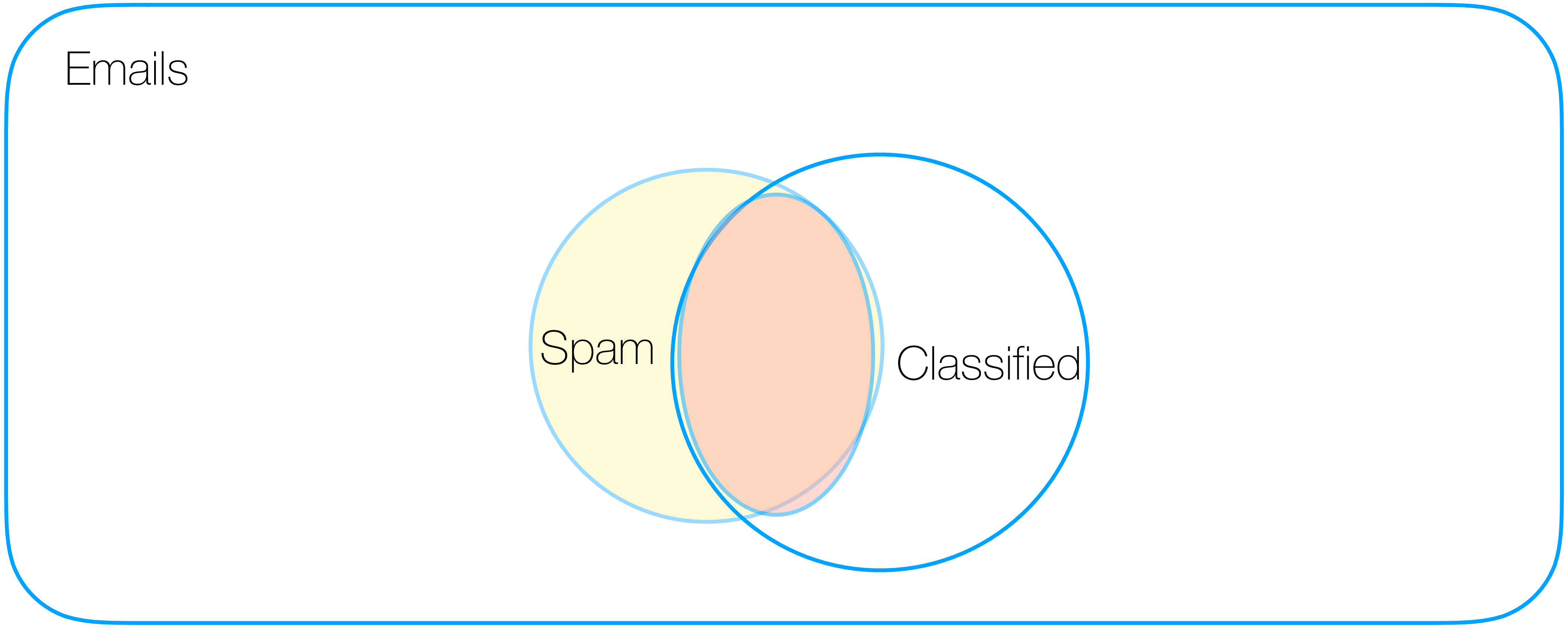

$$p(C|S) = \frac{S \cap C}{S}$$

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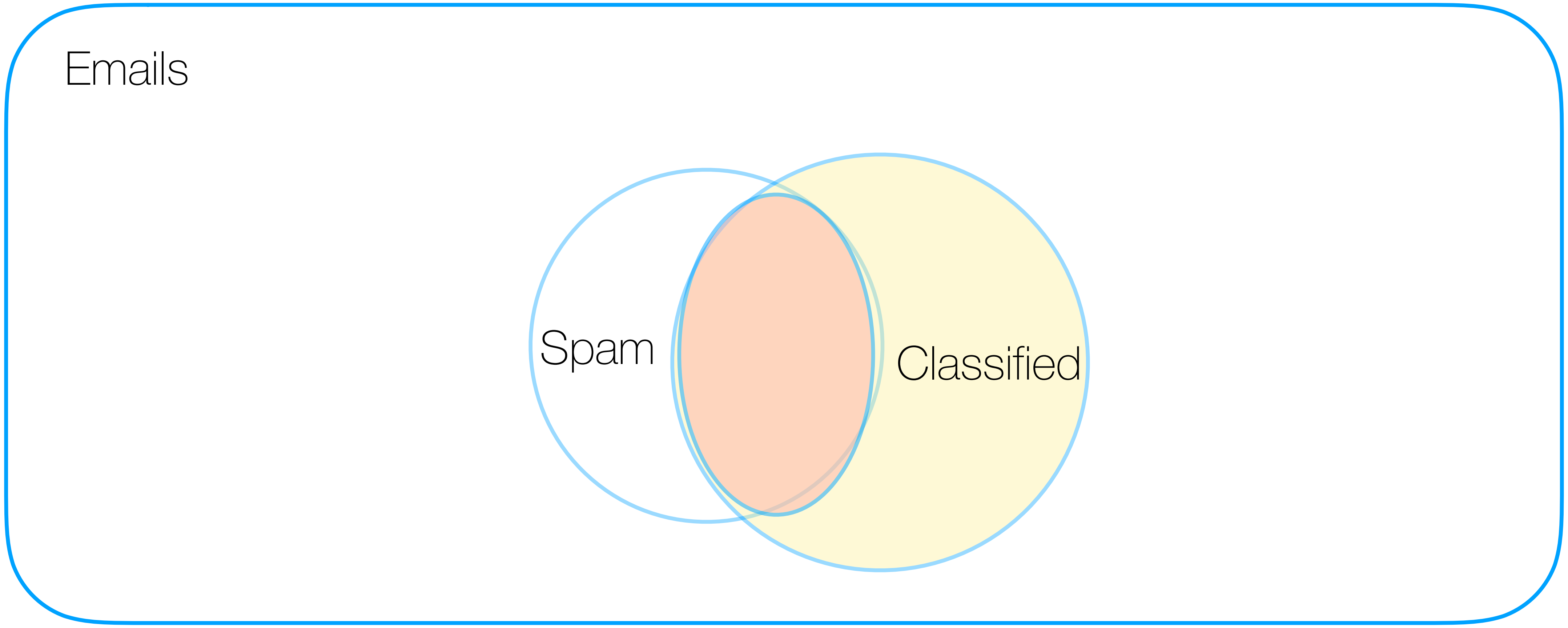

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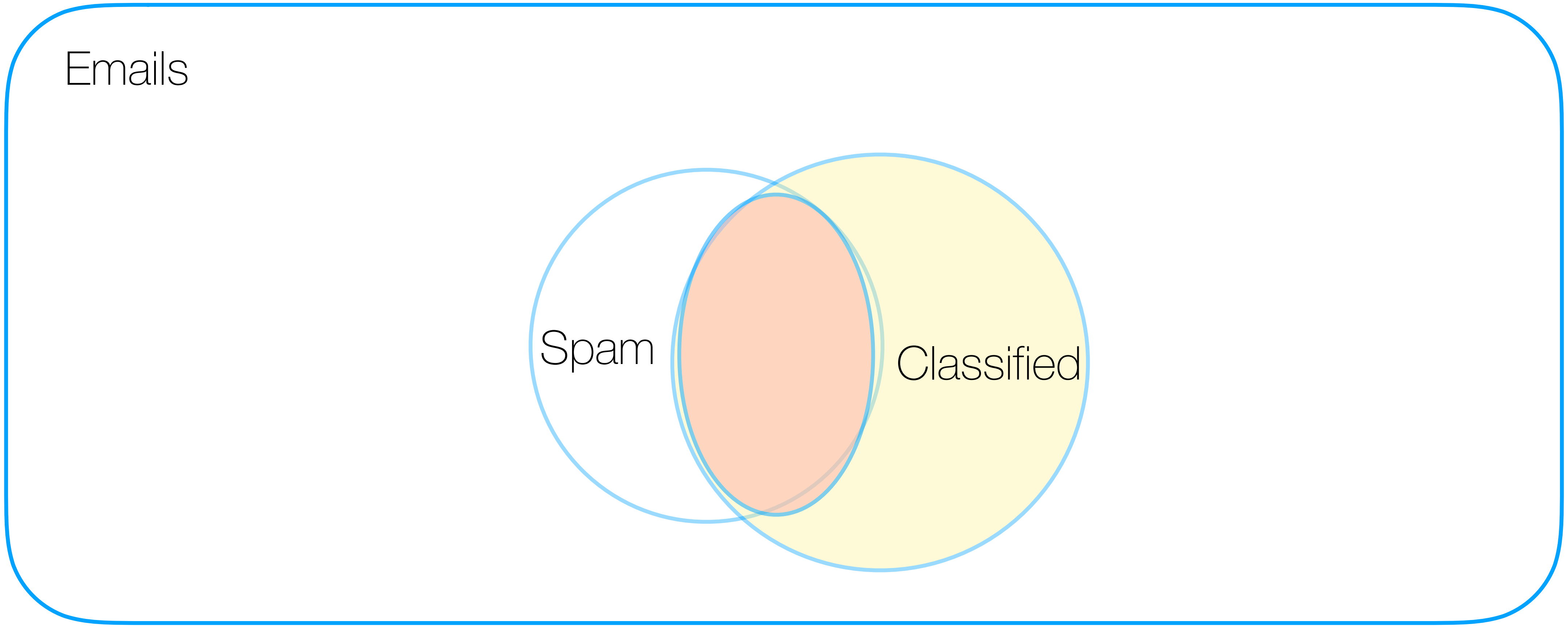

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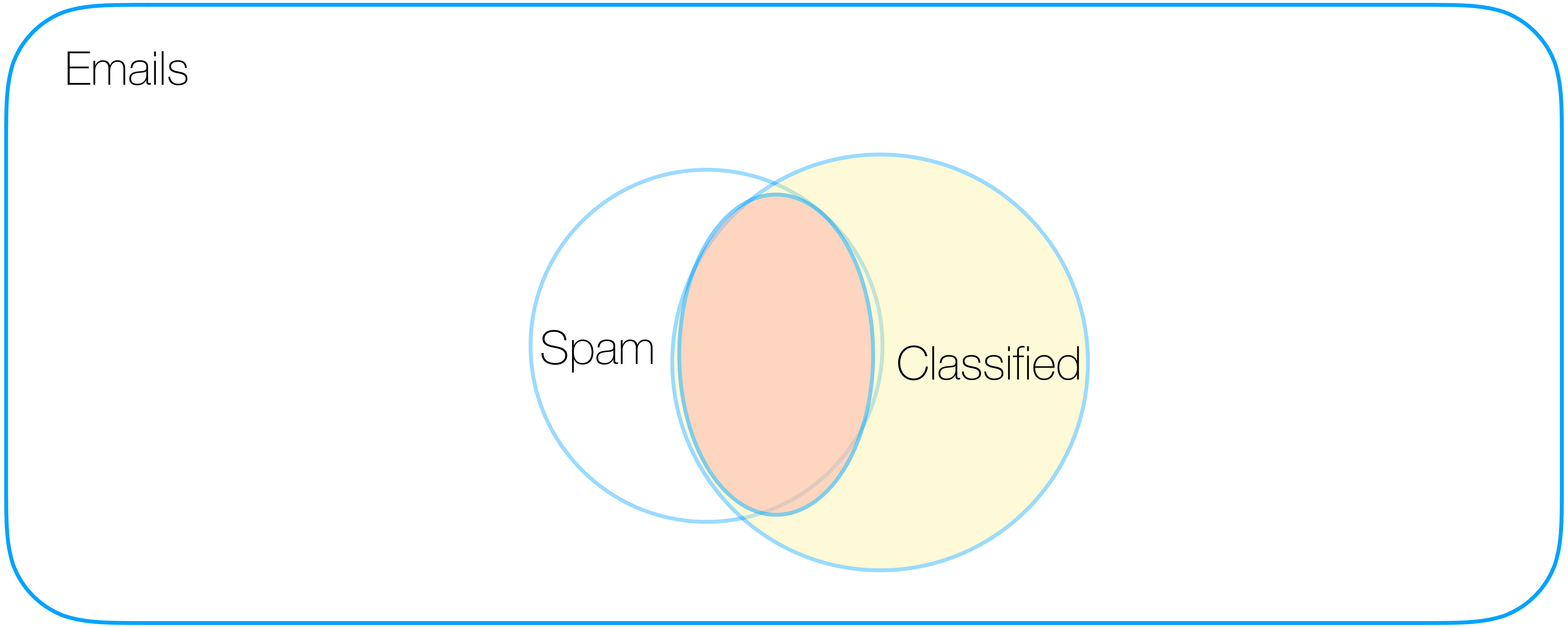

$$p(C|S) = \frac{S \cap C}{S}$$

$$p(S|C) = \frac{S \cap C}{S}\frac{S}{C} = \frac{P(C|S)P(S)}{P(C)}$$

Independent Random Variables

Two random variables *X* and *Y* are *independent* iff measuring *X* gives no information on *Y*, and vice versa.

- Formally: *X* and *Y* are called independent if

  for all $x \in \mathcal{X},\ y \in \mathcal{Y}$

- Equivalent to

$$p(x|y) =$$

- Example:

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- Example:

Throwing two dices

Expectations

- random variable $X \in \mathcal{X}$ and function $f : \mathcal{X} \to \mathbb{R}$

$$\mathbb{E}[f] = \mathbb{E}_{x \sim p(X)}[f(x)] =$$

- For *N* points drawn from p(X):

$$\mathbb{E}[f] =$$

- Conditional expectation:

$$\mathbb{E}[f \,|\, y] = \mathbb{E}_{x \sim p(X|Y=y)}[f(x)]$$

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Variance

- The expected quadratic distance between f and its mean $\mathbb{E}[f]$

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

Variance

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$$
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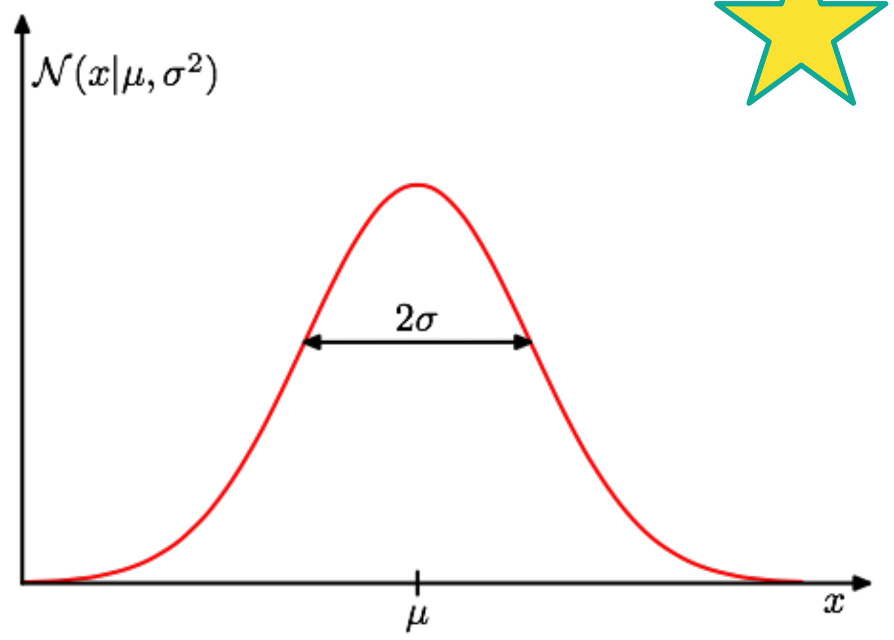
&= E\left[f(x)^2\right] - 2E[f(x)]E[f(x)] + E[f]^2 \\
&= E\left[f(x)^2\right] - E[f(x)]^2
\end{aligned}
$$

Gaussian Distribution



- Real valued stochastic variable *X*

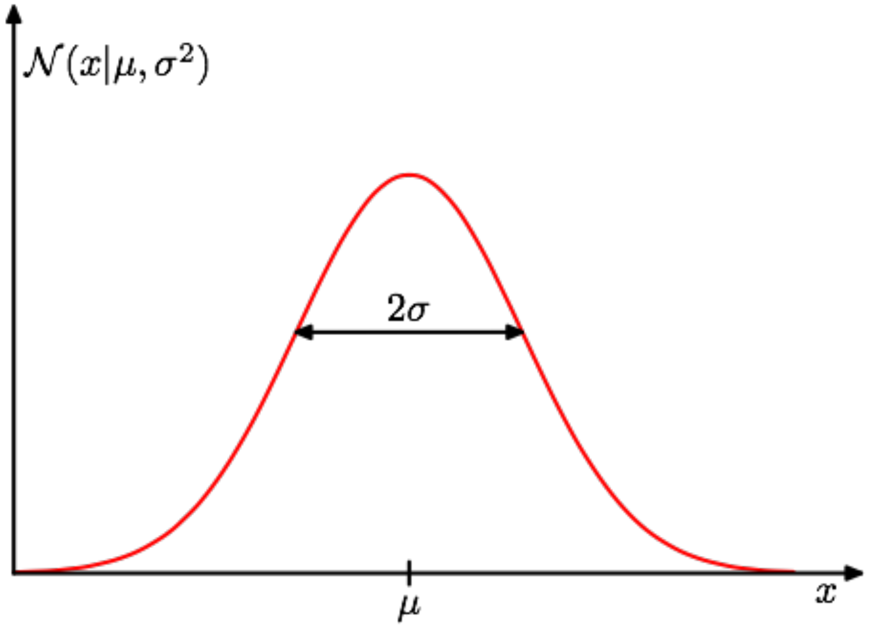
$$\mathcal{N}(x|\mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\{-\frac{1}{2\sigma^2}(x-\mu)^2\}$$

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

- Variance: $\mathrm{var}[x] = \mathbb{E}[(x - \mathbb{E}[x])^2] = ?$

Gaussian Distribution

- Real valued stochastic variable *X*



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$$\boxed{\int_{-\infty}^{\infty} y e^{-y^2} \mathrm{d}y = 0}$$

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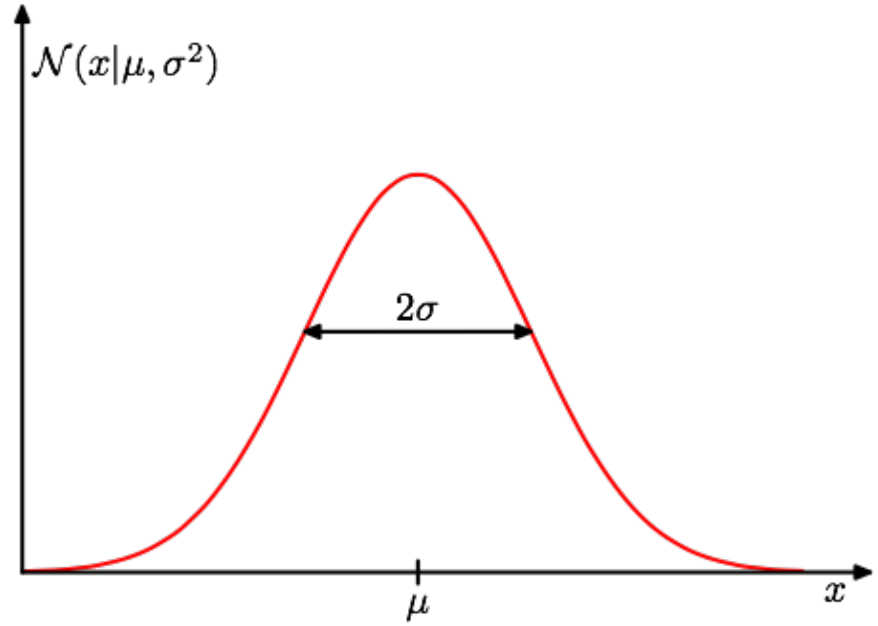
Gaussian Distribution

- Real valued stochastic variable *X*



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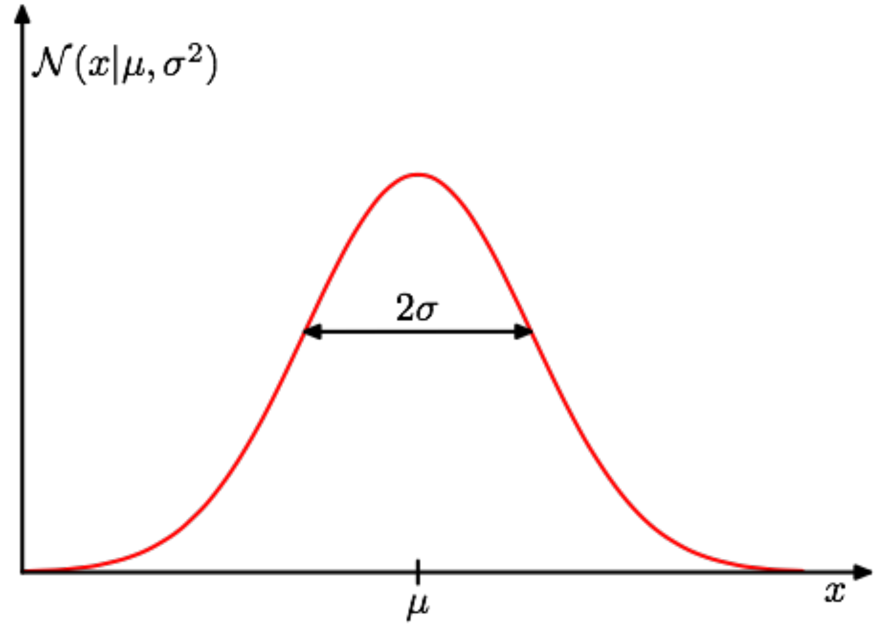

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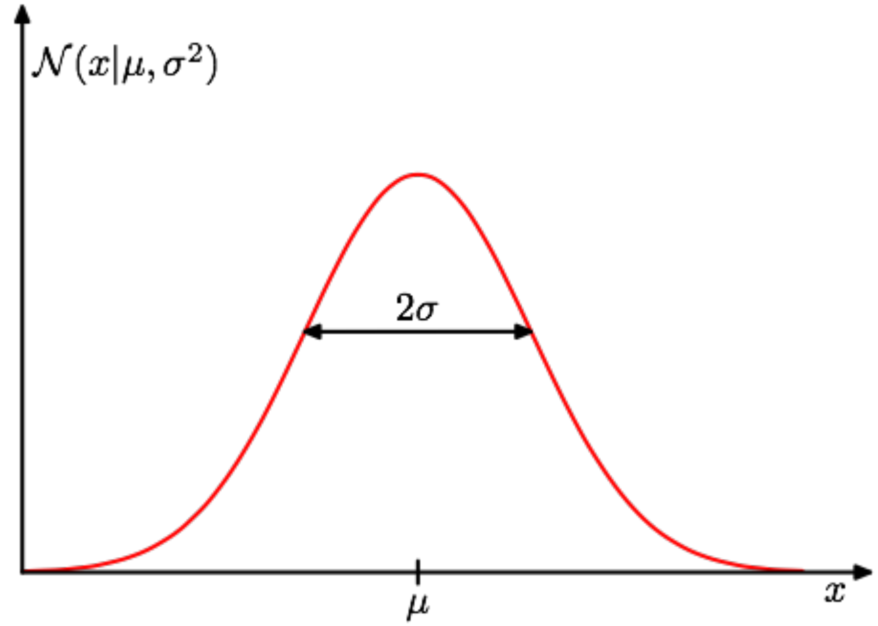

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$$y = \frac{1}{\sqrt{2\sigma^2}}(x-\mu)$$

$$\downarrow$$

$$x = \mu + y\sqrt{2\sigma^2}$$

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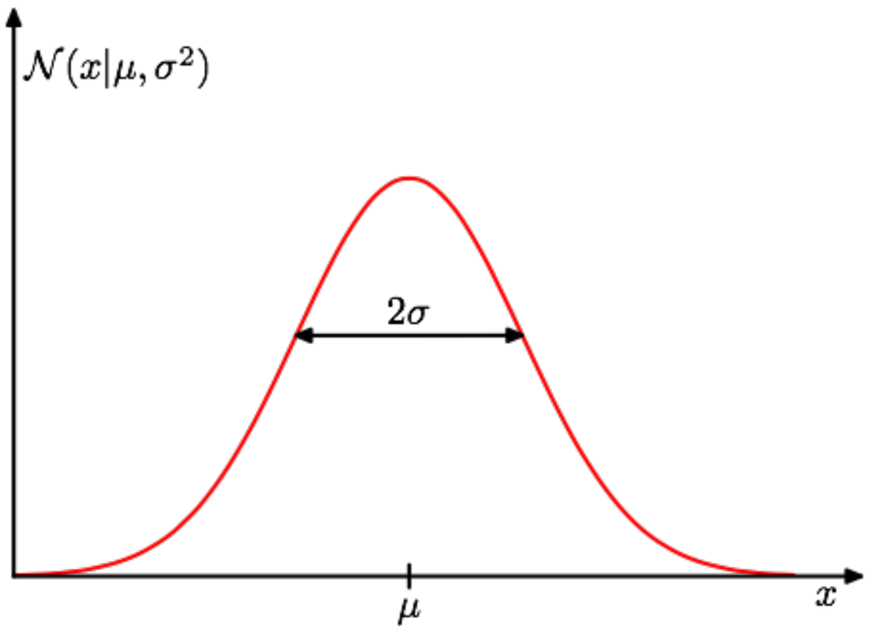

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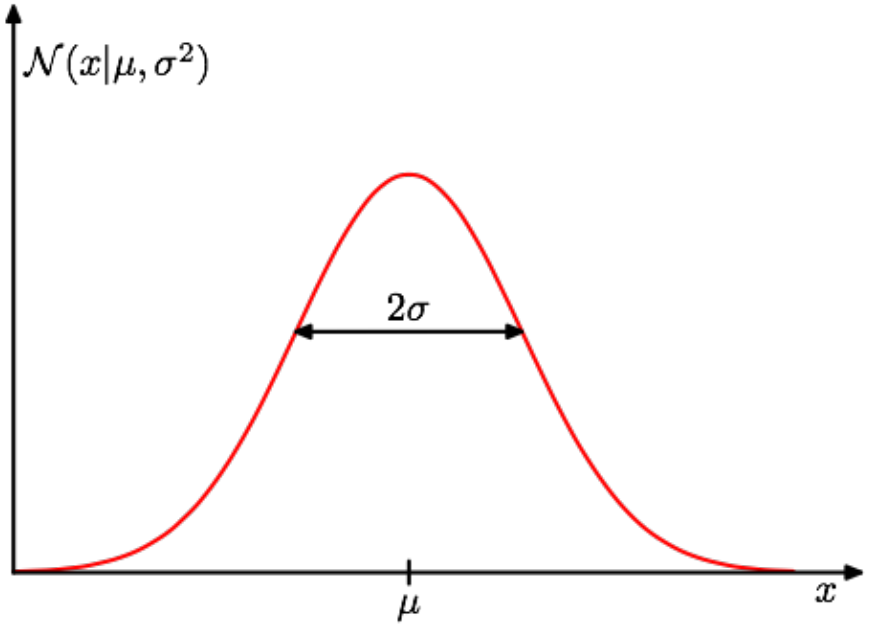

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$$= \int_{-\infty}^{\infty} \frac{\mu + y\sqrt{2\sigma^2}}{\sqrt{2\pi\sigma^2}} e^{-y^2}\sqrt{2\sigma^2}dy \;= \frac{\mu\sqrt{2\sigma^2}}{\sqrt{2\pi\sigma^2}}\int_{-\infty}^{\infty} e^{-y^2}dy + \frac{2\sigma^2}{\sqrt{2\pi\sigma^2}}\int_{-\infty}^{\infty} ye^{-y^2}$$

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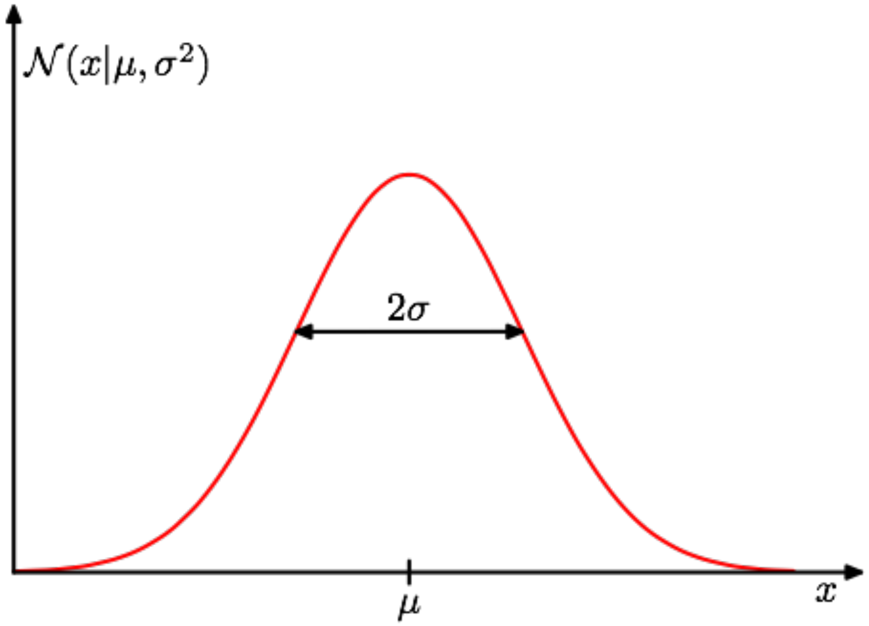

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$$= \int_{-\infty}^{\infty}\frac{\mu + y\sqrt{2\sigma^2}}{\sqrt{2\pi\sigma^2}}e^{-y^2}\sqrt{2\sigma^2}dy = \frac{\mu\sqrt{2\sigma^2}}{\sqrt{2\pi\sigma^2}}\int_{-\infty}^{\infty}e^{-y^2}dy + \frac{2\sigma^2}{\sqrt{2\pi\sigma^2}}\int_{-\infty}^{\infty}ye^{-y^2}$$

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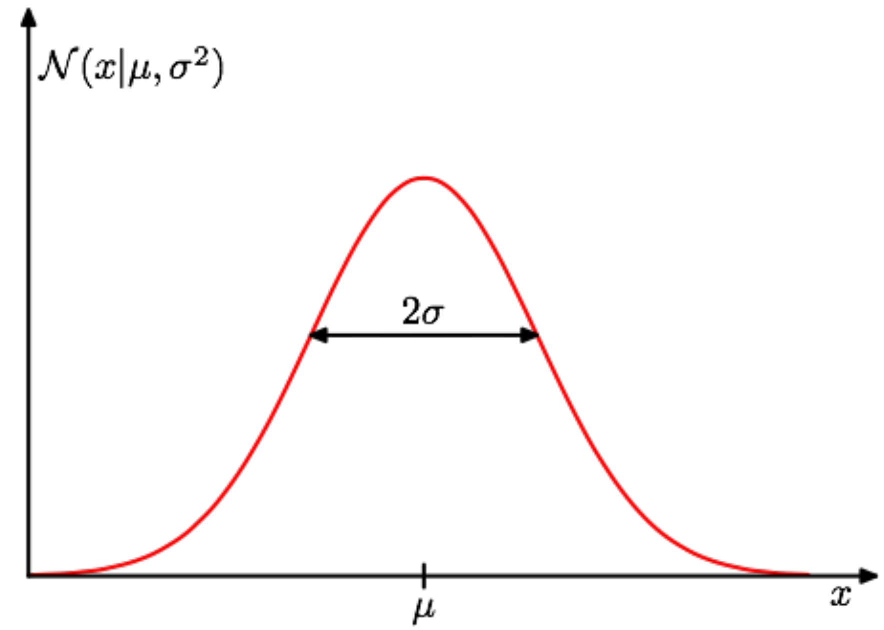
Gaussian Distribution



- Real valued stochastic variable *X*

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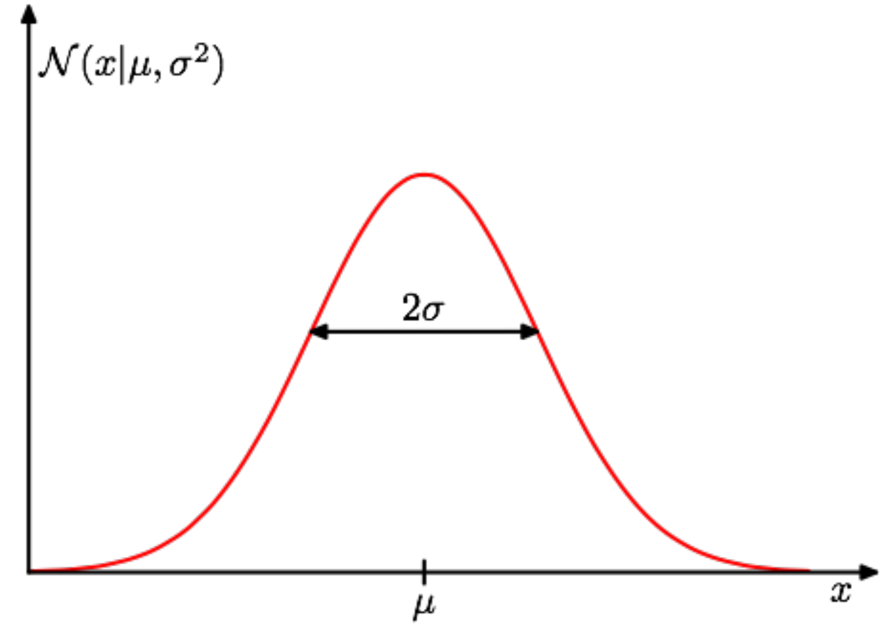

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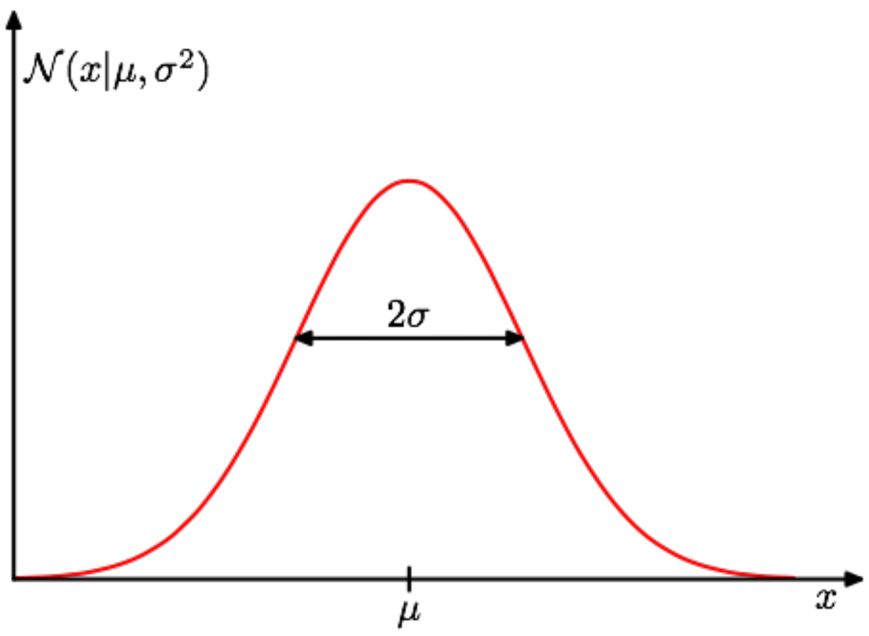

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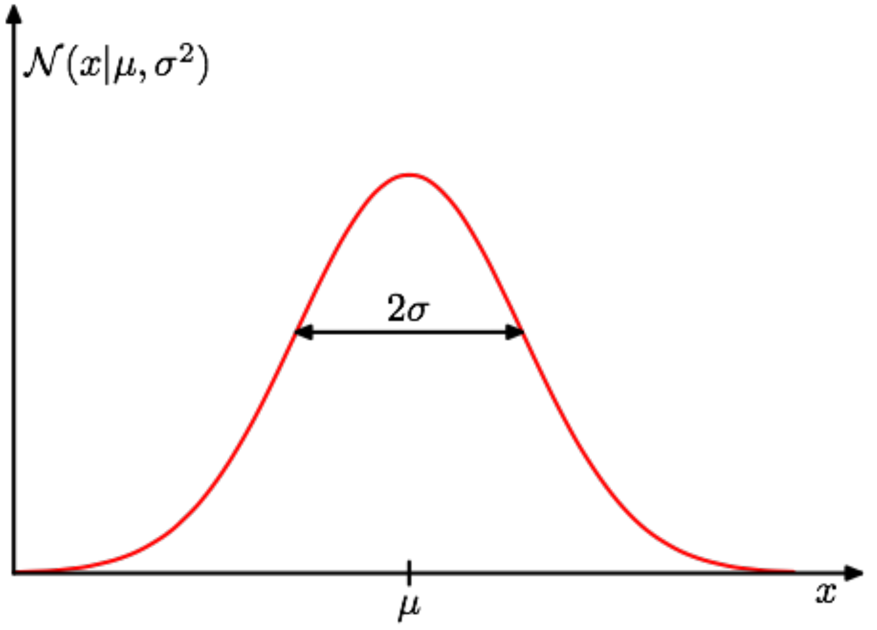

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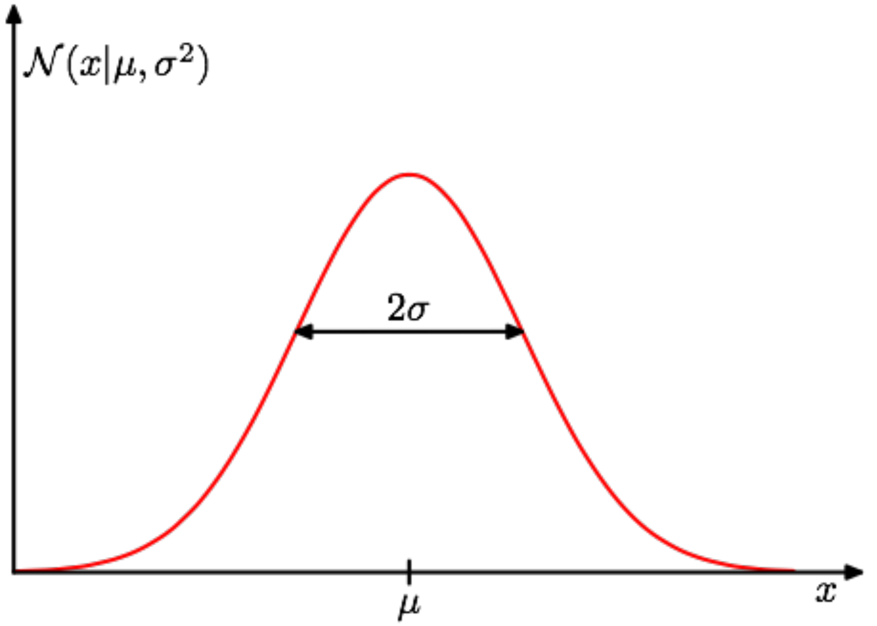

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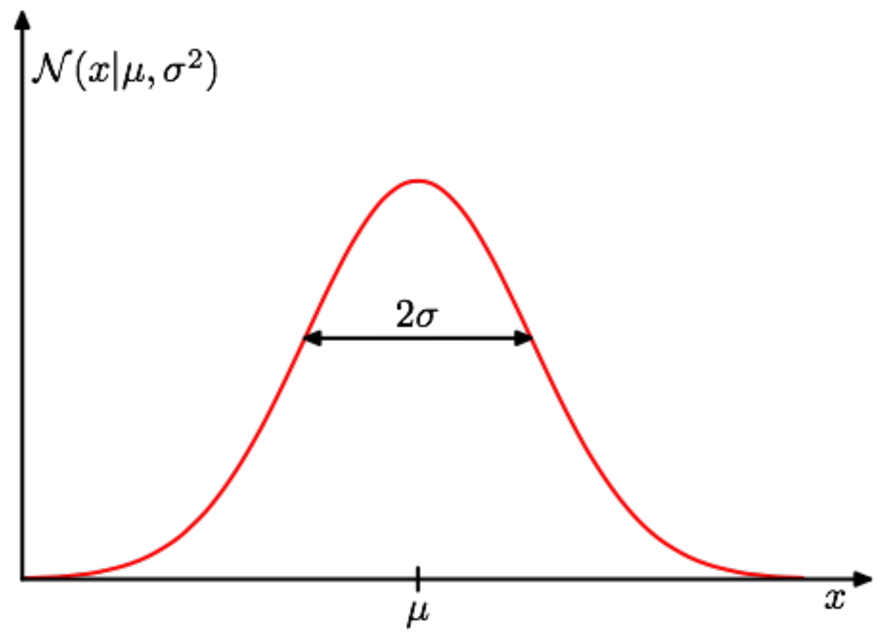

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Multivariate Gaussian Distribution

- *D*-dimensional vector $\mathbf{x} = (x_1, x_2, ..., x_D)^T$
- $\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) =$

$|\boldsymbol{\Sigma}| = \det \boldsymbol{\Sigma}$

- $\boldsymbol{\Sigma} =$

(D x D matrix)

- $\mathbb{E}[\mathbf{x}] =$

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Exercises with Gaussians

- Compute:
- Mean of uni-/multivariate Gaussian (-> mu)
- Variance of univariate Gaussian (-> sigma)
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- Integral: $\int_{-\infty}^{+\infty} e^{-x^2} dx = \sqrt{\pi}$
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Overview

1. Probability theory

2. **Statistical learning principles:**

    I. **Maximum likelihood**

    II. Maximum a posteriori

    III. Bayesian prediction

Maximum Likelihood Estimation

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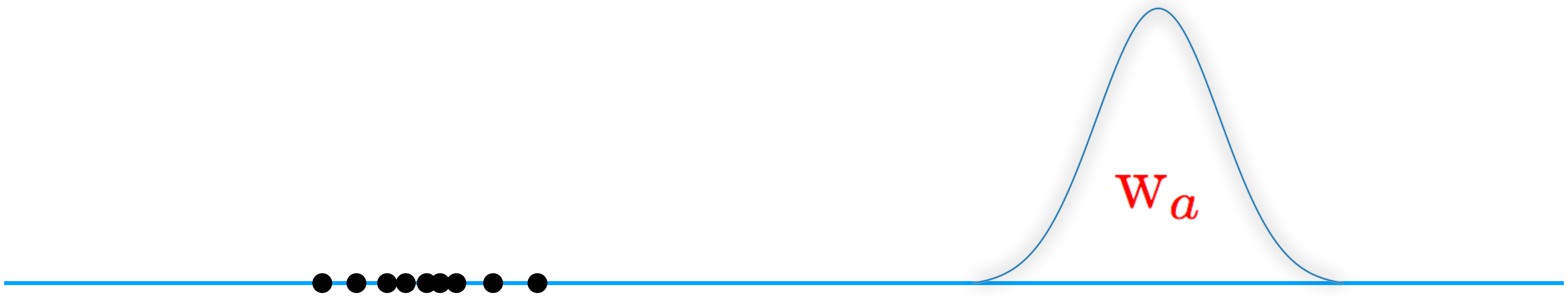

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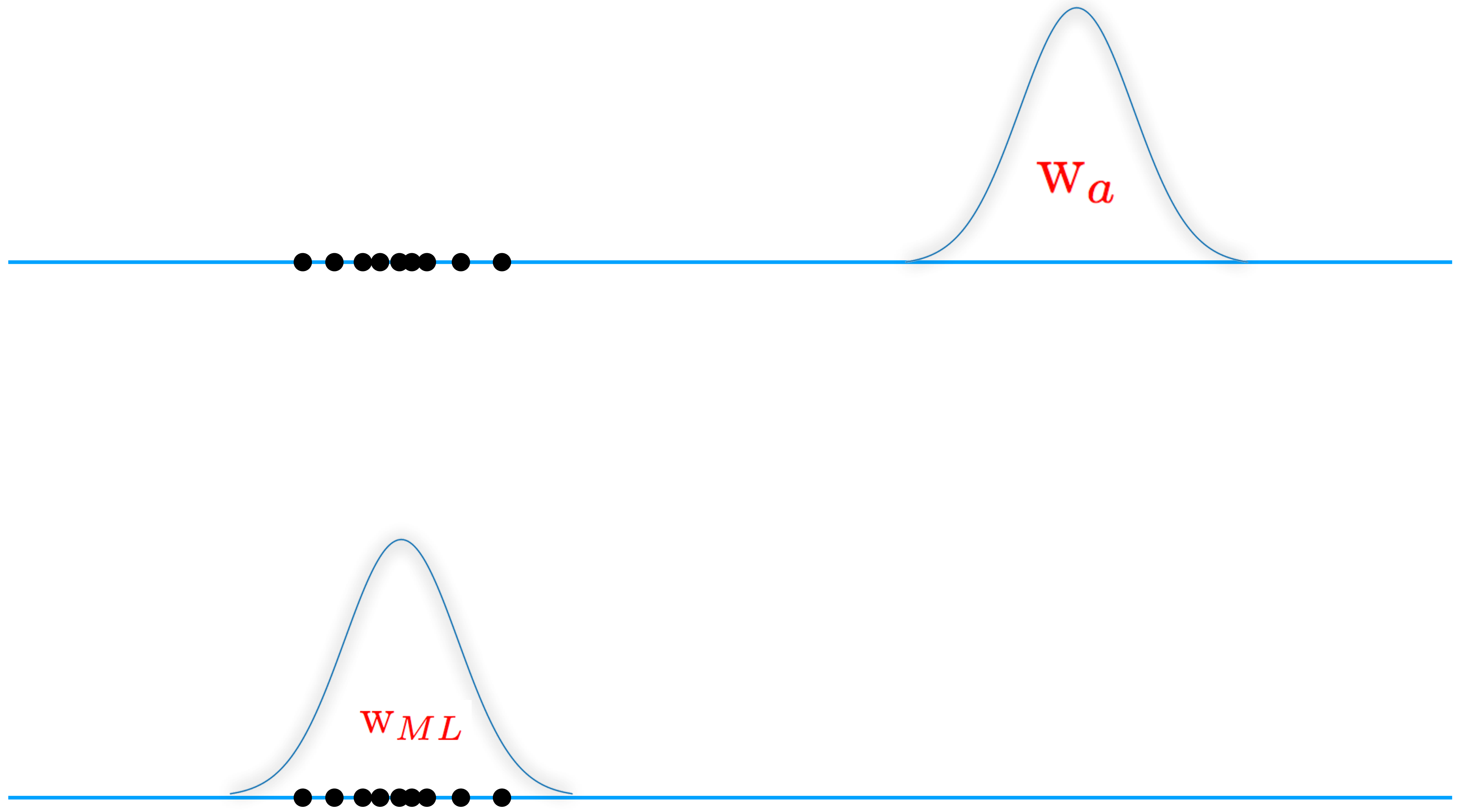

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numerical underflow/overflow

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- Error function: $E(D;\mathbf{w}) = -\log p(D|\mathbf{w}) = -\sum_{i=1}^{N} \log p(x_i|\mathbf{w})$

ML Estimator for Gaussian Distributions (I)

- i.i.d. Gaussian distributed real variables $D = (x_1, x_2, ..., x_N)$

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- Estimate model parameters:

$$\mu_{ML} = ? \qquad \sigma_{ML} = ?$$

ML Estimator for Gaussian Distributions (II)

- log likelihood:

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- Maximum Likelihood solution for μ

$$\frac{\partial}{\partial \mu} \log p(D|\mu, \sigma^2) =$$

ML Estimator for Gaussian Distributions (II)

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$$\mu = \frac{1}{N}\sum_{i=1}^{N}x_i$$

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- Maximum Likelihood solution for σ^2

$$\frac{\partial}{\partial\sigma^2}\log p(D|\mu,\sigma^2) = \textcolor{red}{0}$$

ML Estimator for Gaussian Distributions (II)

- log likelihood:

$$\log p(D|\mu, \sigma^2) = -\frac{N}{2} \log 2\pi\sigma^2 - \frac{1}{2\sigma^2} \sum_{i=1}^{N} (x_i - \mu)^2$$

- Maximum Likelihood solution for σ^2

$$\frac{\partial}{\partial \sigma^2} \log p(D|\mu, \sigma^2) = 0$$

$$\sigma^2_{ML} = \frac{1}{N} \sum_{i=1}^{N} (x_i - \mu)^2$$

ML Estimator for Gaussian Distributions (IV)

- How well do the ML estimators represent the true parameters? $$p(D|\mu,\sigma^2) = \frac{1}{(2\pi\sigma^2)^{N/2}} \prod_{i=1}^{N} \exp\left[-\frac{1}{2\sigma^2}(x_i-\mu)^2\right]$$
- If I draw multiple datasets, what is the expected value of μ_{ML}?
- ML estimate of the mean:

$$\mathbb{E}_{D\sim p(D|\mu,\sigma^2)}[\mu_{\mathrm{ML}}] = \mathbb{E}\left[\frac{1}{N}\sum_{i=1}^{N} x_i\right] =$$

- Bias of estimator:

$$\mathbb{E}[\mu_{\mathrm{ML}}] - \mu$$

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ML Estimator for Gaussian Distributions (V)

- ML estimate of the variance:

$$\mathbb{E}_{D \sim p(D|\mu,\sigma^2)}[\sigma^2_{ML}] = \mathbb{E}\left[\frac{1}{N}\sum_{i=1}^{N}\left(x_i - \frac{1}{N}\sum_{n=1}^{N}x_n\right)^2\right] =$$

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$$\cdots = \sigma^2(\frac{N-1}{N})$$

ML Estimator for Gaussian Distributions (VI)

- For data generated from

$$p(D|\mu,\sigma^2) = \frac{1}{(2\pi\sigma^2)^{N/2}} \prod_{i=1}^{N} \exp\left[-\frac{1}{2\sigma^2}(x_i-\mu)^2\right]$$

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$$\mathbb{E}[\sigma^2_{\mathrm{ML}}] = \quad \cdots = \sigma^2\left(\frac{N-1}{N}\right)$$

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Biased Maximum Likelihood Estimator

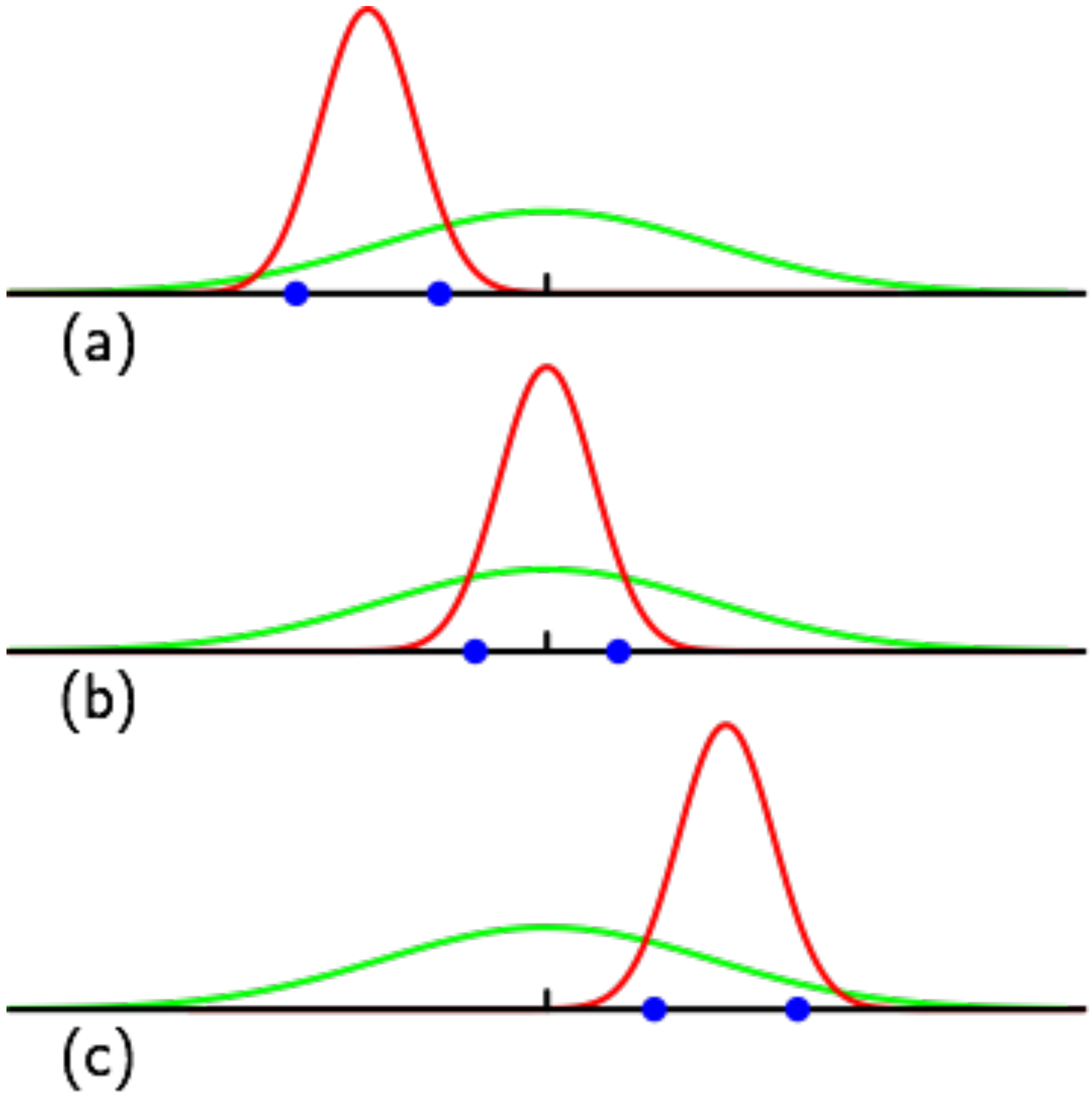

Figure: Bias in ML estimator for variance (Bishop 1.15)

Curve Fitting: Maximum Likelihood Estimates

- Data $D = \{(x_1, t_1), ..., (x_N, t_N)\} = \{\mathbf{x}, \mathbf{t}\}$

- Assume targets are generated by

$$t = y(x, \mathbf{w}) + \sigma\varepsilon, \quad \varepsilon \sim \mathcal{N}(\varepsilon|0, 1)$$

- Target distribution:

$$p(t|x, \mathbf{w}, \beta) =$$

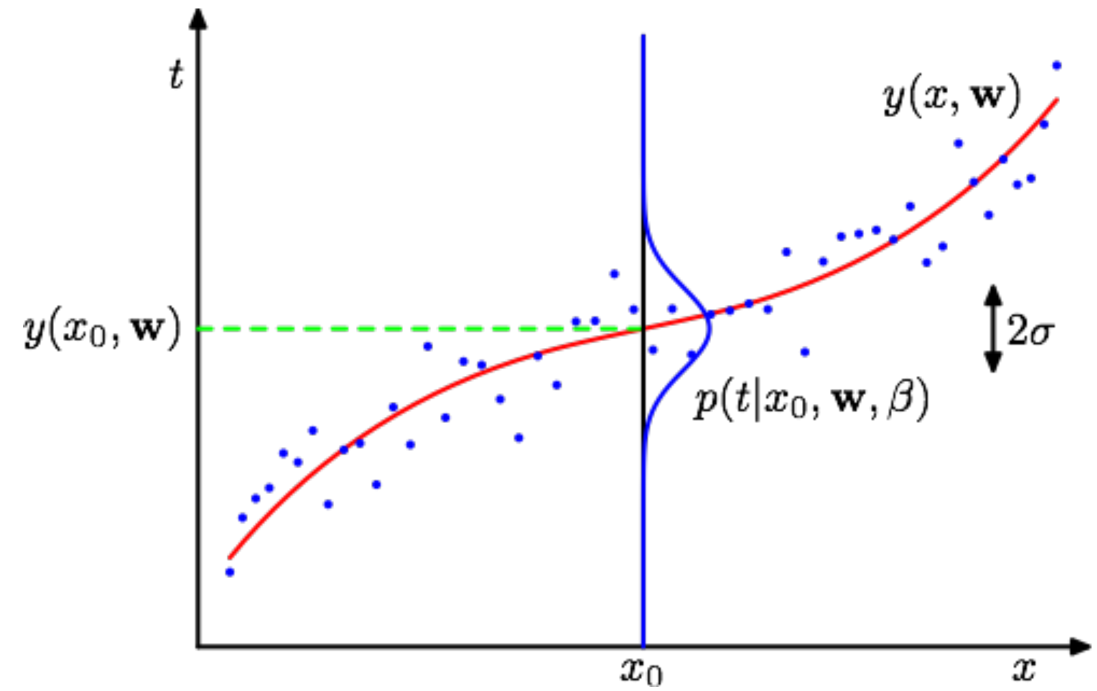

Figure: Gaussian conditional distribution (Bishop 1.16)

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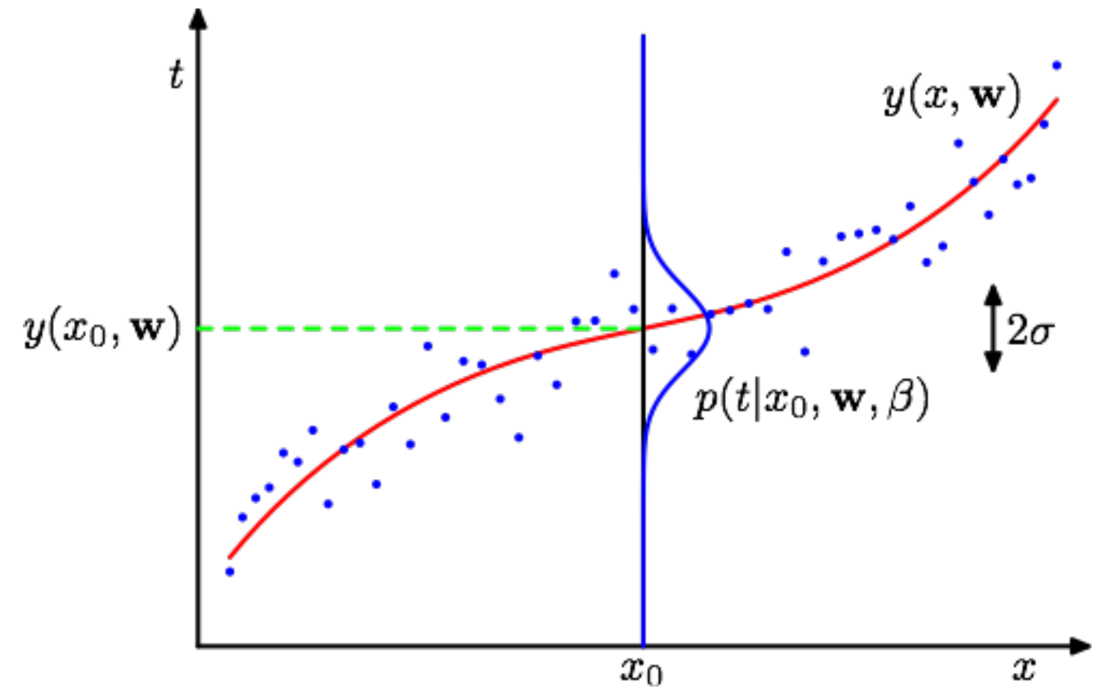

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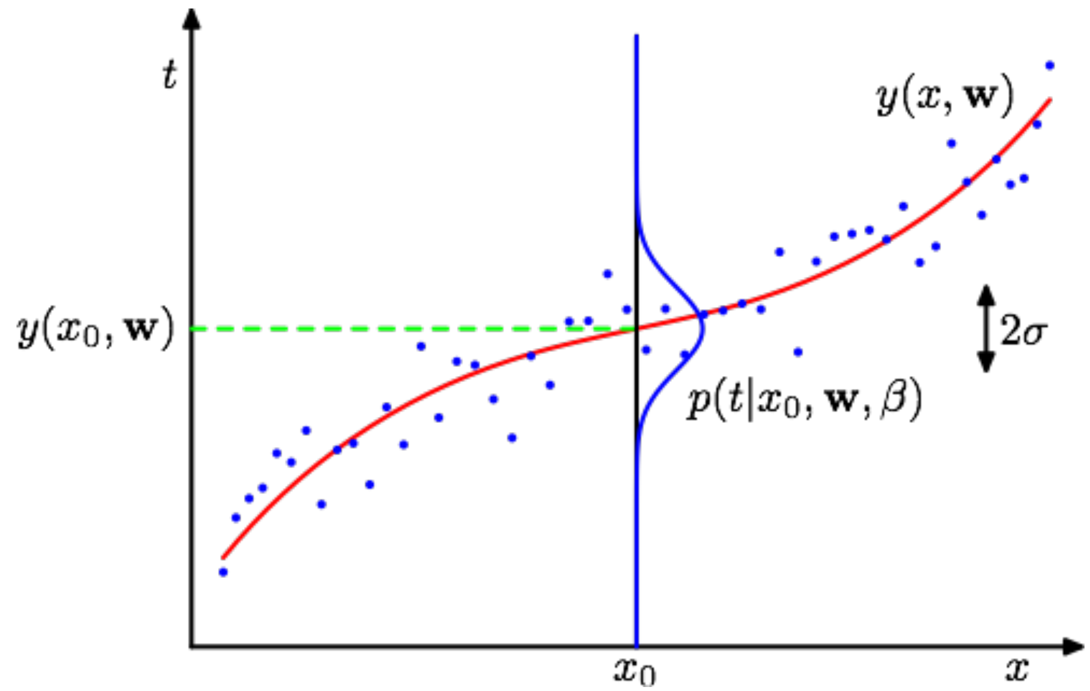

Figure: Gaussian conditional distribution (Bishop 1.16)

- Target distribution:

$$p(t|x, \mathbf{w}, \beta) = \mathcal{N}(t|y(x, \mathbf{w}), \beta^{-1}) = \frac{1}{\sqrt{2\pi\beta^{-1}}} e^{-\frac{\beta}{2}(t - y(x, \mathbf{w}))^2}$$

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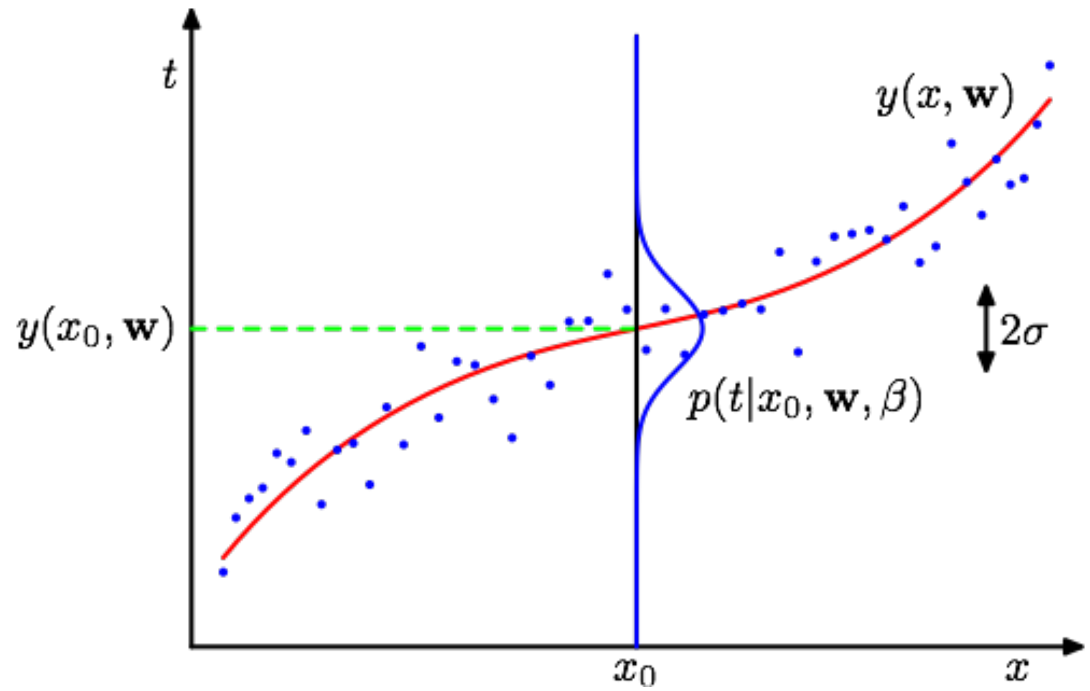

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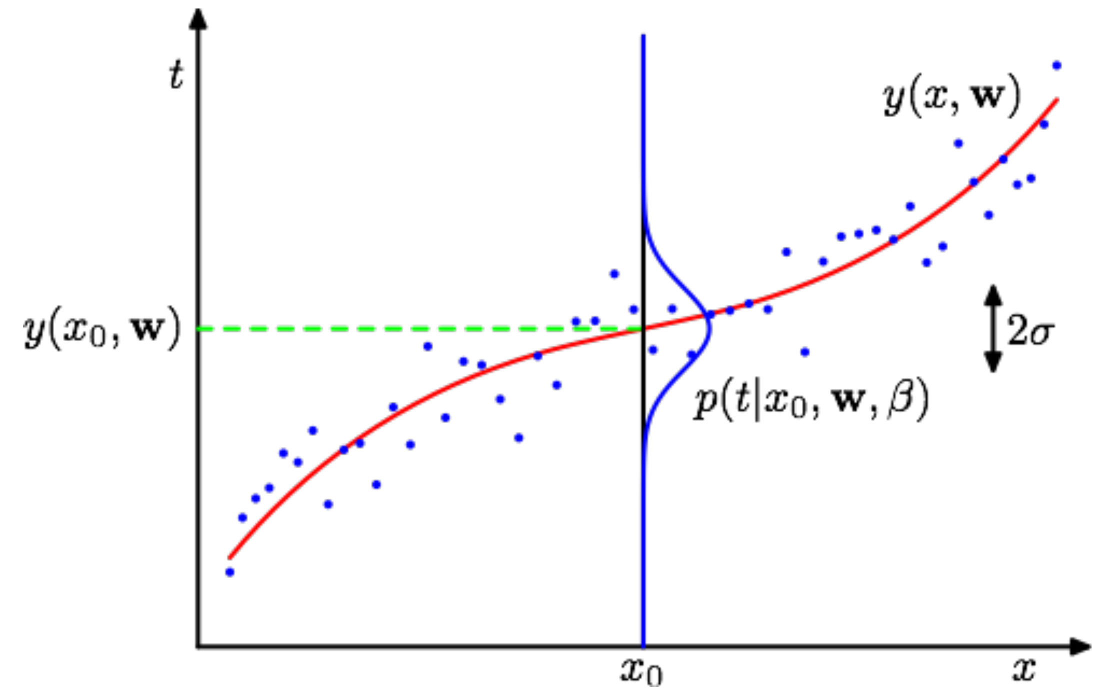

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- Log likelihood:

$$\log p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta) = log \prod_{i=1}^{N} \mathcal{N}(t_i|y(x_i, \mathbf{w}), \beta^{-1})$$

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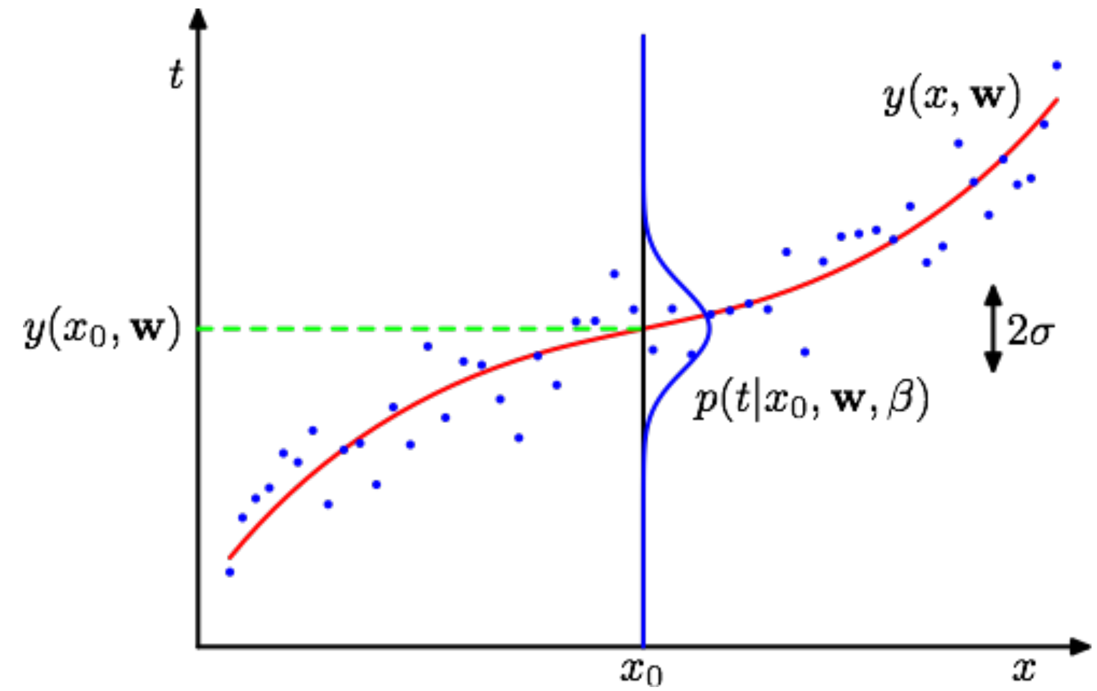

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- Log likelihood:

$$\log p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta) = log \prod_{i=1}^{N} \mathcal{N}(t_i|y(x_i, \mathbf{w}), \beta^{-1}) = -\frac{\beta}{2} \sum_{i=1}^{N} (y(x_i, \mathbf{w}) - t_i)^2 + \frac{N}{2} \log \beta - \frac{N}{2} \log 2\pi$$

Curve Fitting: Maximum Likelihood Estimates

- ML: minimize $E(\mathbf{x}, \mathbf{t}, \mathbf{w}, \beta) = -\log p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta)$ w.r.t. ***w*** and $\boldsymbol{\beta}$

$$E(\mathbf{x}, \mathbf{t}, \mathbf{w}, \beta) = \frac{\beta}{2} \sum_{i=1}^{N} (y(x_i, \mathbf{w}) - t_i)^2 - \frac{N}{2} \log \beta + \frac{N}{2} \log 2\pi$$

- Maximum likelihood solution:

$$\mathbf{w}_{\text{ML}} = \arg\min_{\mathbf{w}} \frac{\beta}{2} \sum_{i=1}^{N} (y(x_i, \mathbf{w}) - t_i)^2$$

$$\frac{1}{\beta_{\text{ML}}} =$$

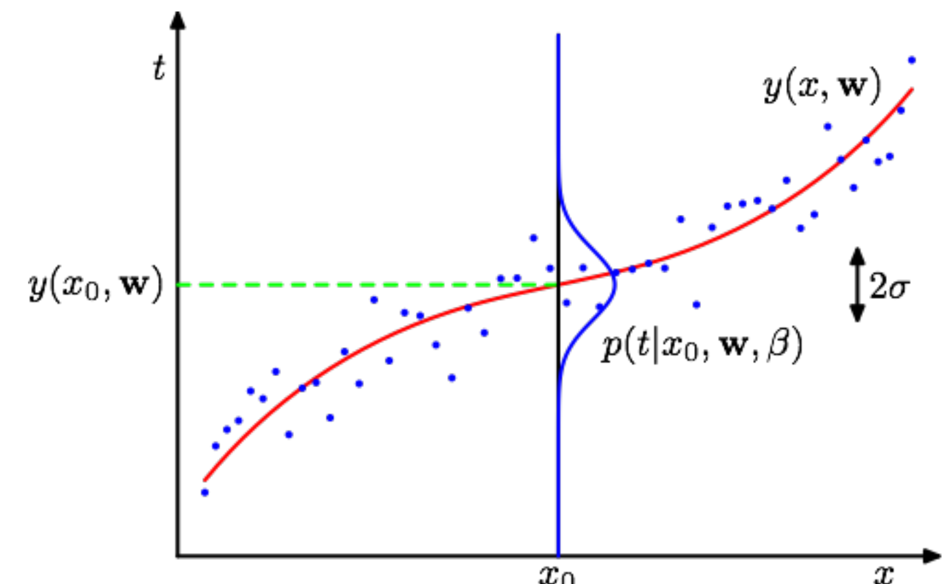

Figure: Gaussian conditional distribution (Bishop 1.16)

Curve Fitting: Maximum Likelihood Estimates

- ML: minimize $E(\mathbf{x}, \mathbf{t}, \mathbf{w}, \beta) = -\log p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta)$ w.r.t. ***w*** and $\boldsymbol{\beta}$

$$E(\mathbf{x}, \mathbf{t}, \mathbf{w}, \beta) = \frac{\beta}{2} \sum_{i=1}^{N} (y(x_i, \mathbf{w}) - t_i)^2 - \frac{N}{2} \log \beta + \frac{N}{2} \log 2\pi$$

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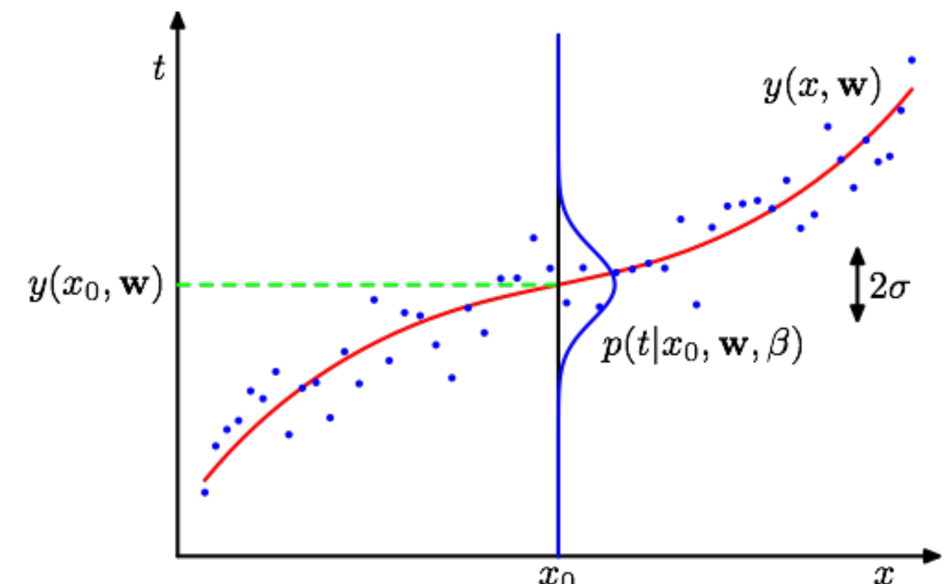

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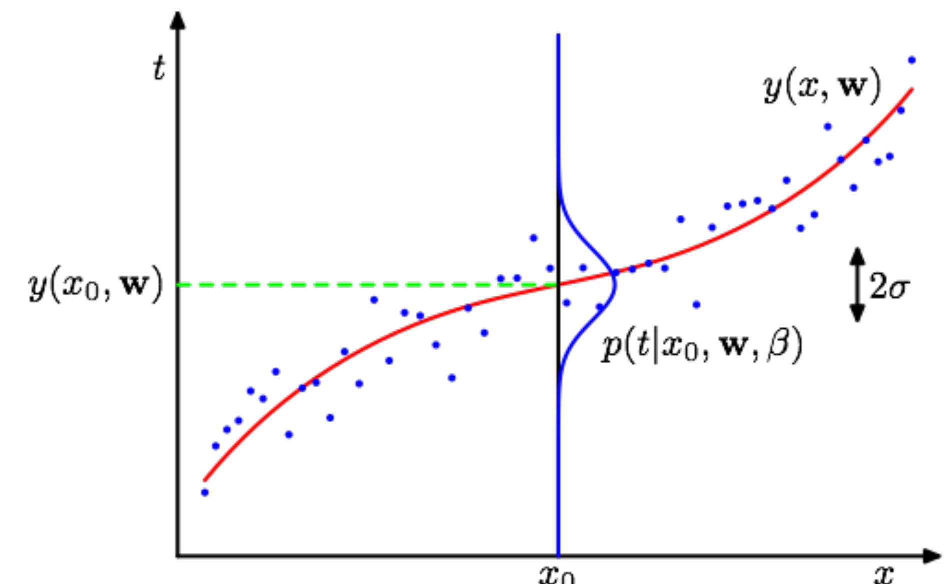

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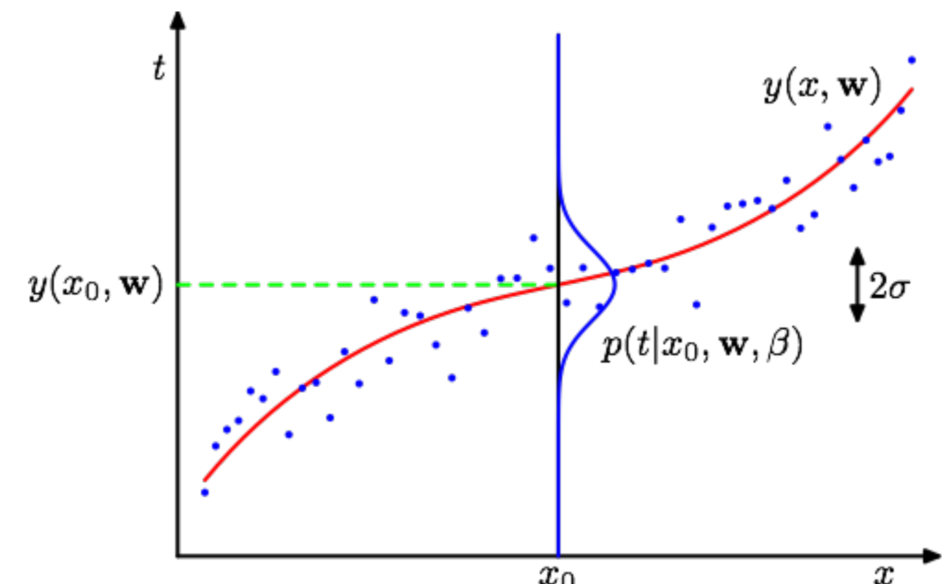

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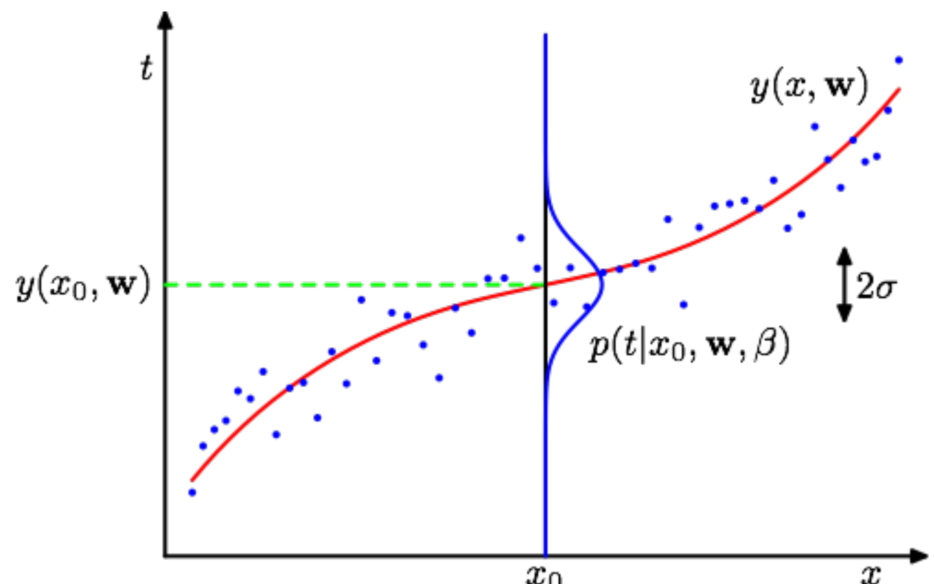

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Overview

1. Probability theory

2. **Statistical learning principles:**

   I. Maximum likelihood

   II. Maximum a posteriori

   III. Bayesian prediction

Maximum A Posteriori Estimates

- Dataset $D = (x_1, x_2, \ldots, x_N)$ of N independent observations.

- ML estimate: choose $\boldsymbol{w}$ such that data likelihood is maximized:

$$\mathbf{w}_{\mathrm{ML}} = \arg\max_{\mathbf{w}} p(D|\mathbf{w})$$

- MAP estimate: choose most probable $\boldsymbol{w}$ given the data.

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- Dataset $D = \{(x_1, t_1), ..., (x_N, t_N)\} = \{\mathbf{x}, \mathbf{t}\}$
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Curve Fitting: Maximum A Posteriori Estimates

- Gaussian prior: $\mathbf{w} \in \mathbb{R}^M$

$$p(\mathbf{w}|\alpha) = \prod_{i=1}^{M} \mathcal{N}(w_i|0, \alpha^{-1}) = (\frac{\alpha}{2\pi})^{M/2} e^{-\frac{\alpha}{2}\mathbf{w}^T\mathbf{w}}$$

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Bayesian Approach

- Dataset $D = (x_1, x_2, \ldots, x_N)$ of N independent observations.

- Frequentist approach: search for one optimal estimate of ***w***

$$\mathbf{w}_{\mathrm{ML}} =$$

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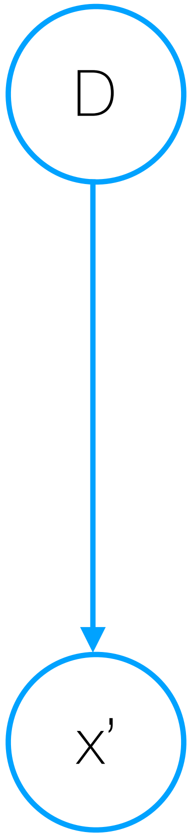
- **Note**: even if $p(D \mid \mathbf{w}) = \prod_{i=1}^{N} p(x_i \mid \mathbf{w})$

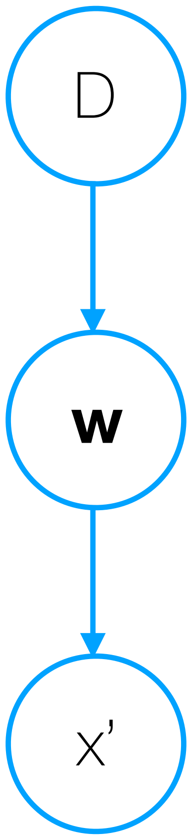
$$p(D) = \int \mathrm{d}\mathbf{w}\, p(D, \mathbf{w}) = \int \mathrm{d}\mathbf{w}\, p(D \mid \mathbf{w}) p(\mathbf{w}) \neq \prod_{i=1}^{N} p(x_i)$$

Curve Fitting: Bayesian Approach



$$p(x' \mid D)$$

Curve Fitting: Bayesian Approach



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

Curve Fitting: Bayesian Approach

- Dataset $D = \{(x_1, t_1), ..., (x_N, t_N)\} = \{\mathbf{x}, \mathbf{t}\}$
- Posterior distribution after observing data:

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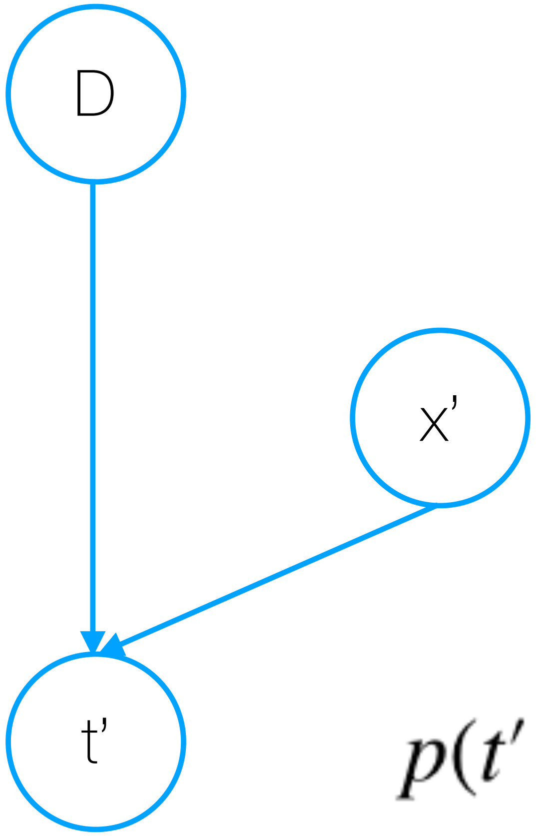
- Predictive distribution:

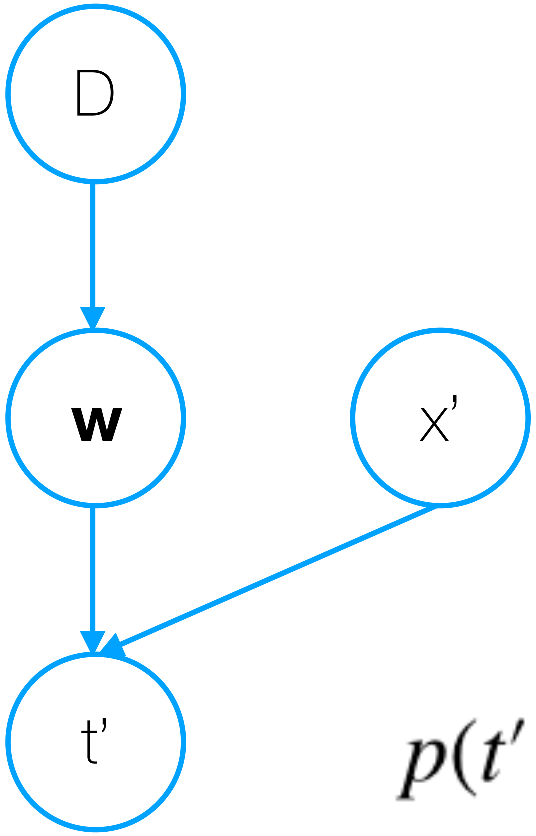
$$p(t' \,|\, x', \mathbf{x}, \mathbf{t}) = \int \mathrm{d}\mathbf{w} p(t', \mathbf{w} \,|\, x', \mathbf{x}, \mathbf{t}) = \int p(t'|x', \mathbf{w})p(\mathbf{w}|\mathbf{x}, \mathbf{t})\mathrm{d}\mathbf{w}$$

Curve Fitting: Bayesian Approach



$$p(t' \mid x', \mathbf{x}, \mathbf{t})$$

Curve Fitting: Bayesian Approach



$$p(t' \mid x', \mathbf{x}, \mathbf{t}) = \int p(t'|x', \mathbf{w})p(\mathbf{w}|\mathbf{x}, \mathbf{t})\mathrm{d}\mathbf{w}$$

Curve Fitting: Bayesian Approach

- Predictive distribution: $p(t'|x', \mathbf{x}, \mathbf{t}) = \int p(t'|x', \mathbf{w})p(\mathbf{w}|\mathbf{x}, \mathbf{t})\mathrm{d}\mathbf{w}$

$$p(\mathbf{w}|\mathbf{x}, \mathbf{t}) = \frac{p(\mathbf{t}|\mathbf{x}, \mathbf{w})p(\mathbf{w})}{p(\mathbf{t}|\mathbf{x})} \quad \text{with} \quad p(\mathbf{t}|\mathbf{x}) = \int p(\mathbf{t}|\mathbf{x}, \mathbf{w})p(\mathbf{w})\mathrm{d}\mathbf{w}$$

Advantages:

- Inclusion of prior knowledge
- Represents uncertainty in ***t'*** both due to target noise, and uncertainty over ***w***.

Disadvantages:

- Posterior is hard to compute analytically → approximate!
- Prior is often chosen for mathematical convenience, not reflection of prior belief!