

Probabilistic Methods-II

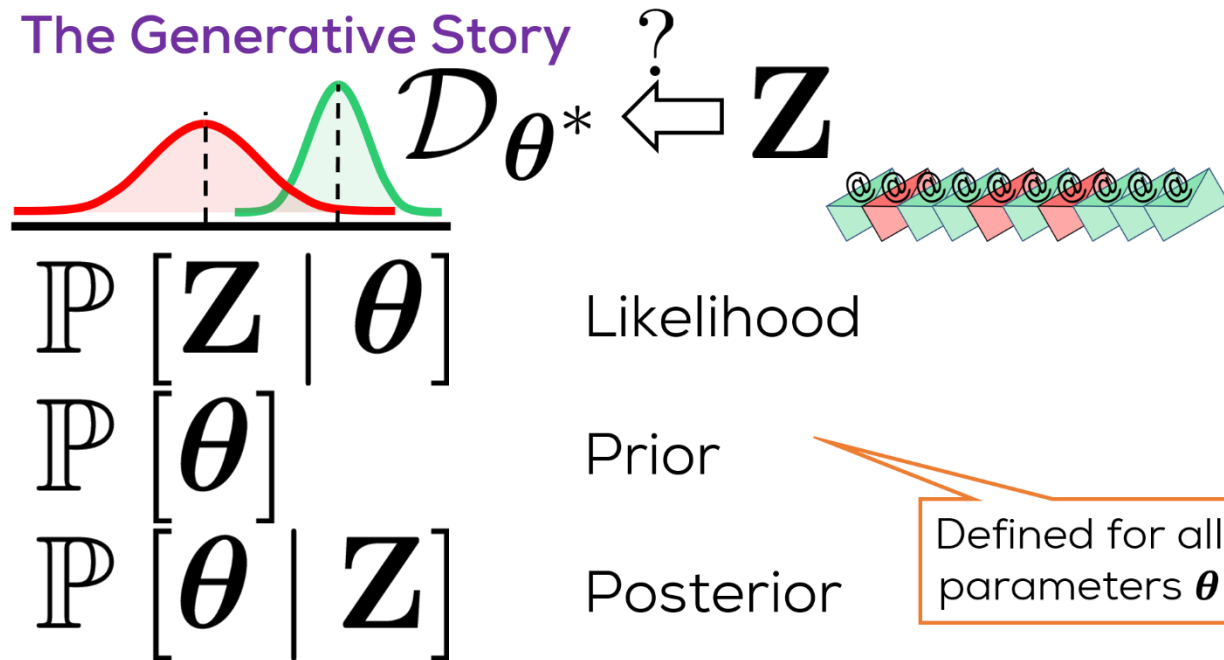
CS771: Introduction to Machine Learning

Purushottam Kar



Recap

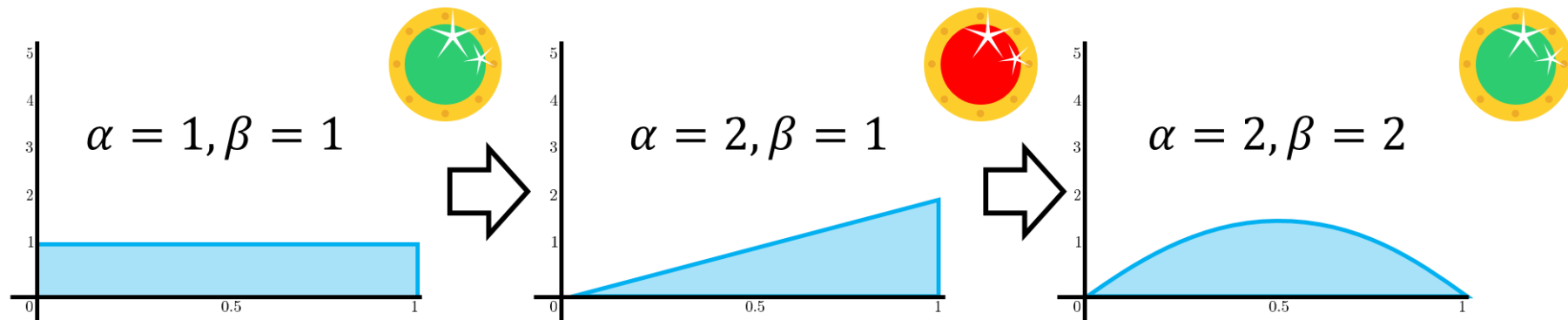
The Generative Story



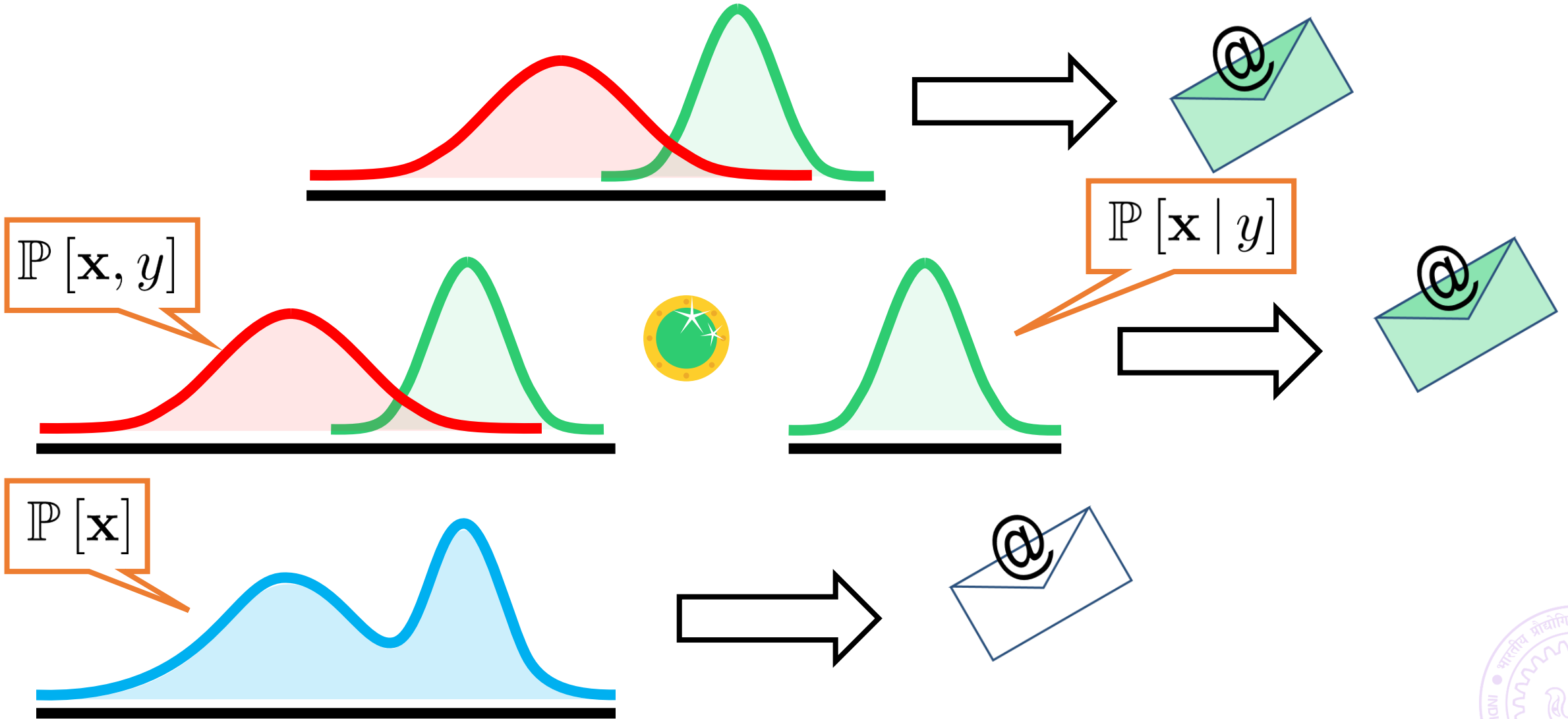
Prediction with learnt models

Diagram illustrating prediction with learnt models. A coin flip is shown with a question mark, representing the prediction of $\mathbf{Z} = \mathbf{y}$ (a sequence of green and red stars). The probability of observing y^i given p is $\mathbb{P}[y^i | p] = p^{y^i} (1 - p)^{1 - y^i}$. The probability of observing \mathbf{y} given p is $\mathbb{P}[\mathbf{y} | p] = \prod_i \mathbb{P}[y^i | p]$. The probability of observing \mathbf{y} given θ is $\mathbb{P}[\mathbf{y} | \theta] = \int \mathbb{P}[\mathbf{y} | p] \mathbb{P}[p | \theta] dp$. The probability of observing \mathbf{y} given \hat{p}_{MLE} is $\mathbb{P}[\mathbf{y} | \hat{p}_{\text{MLE}}] = \frac{n_H}{n}$. The probability of observing \mathbf{y} given \hat{p}_{MAP} is $\mathbb{P}[\mathbf{y} | \hat{p}_{\text{MAP}}] = \frac{n_H + \alpha - 1}{n + \alpha + \beta - 2}$.

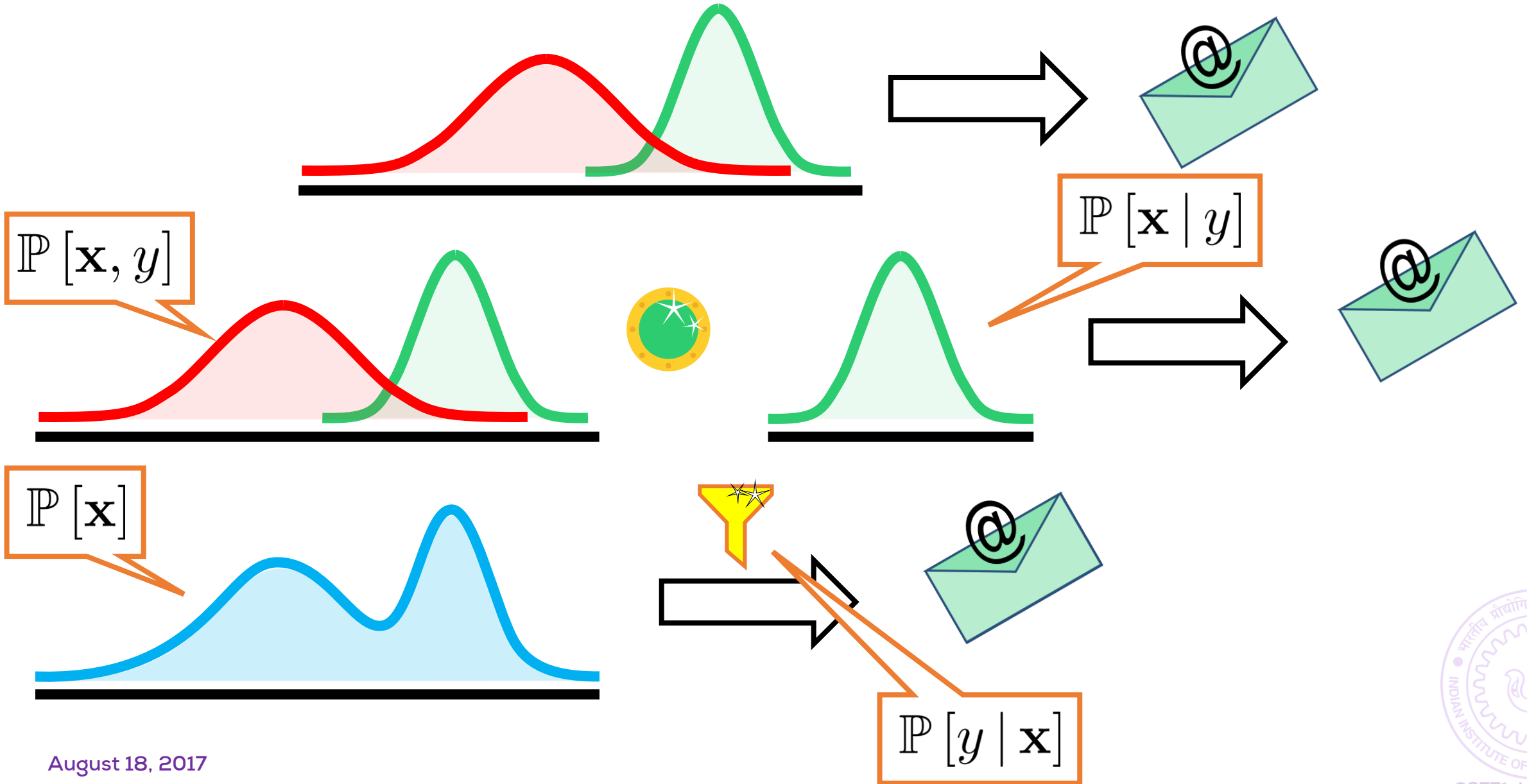
Online MAP!



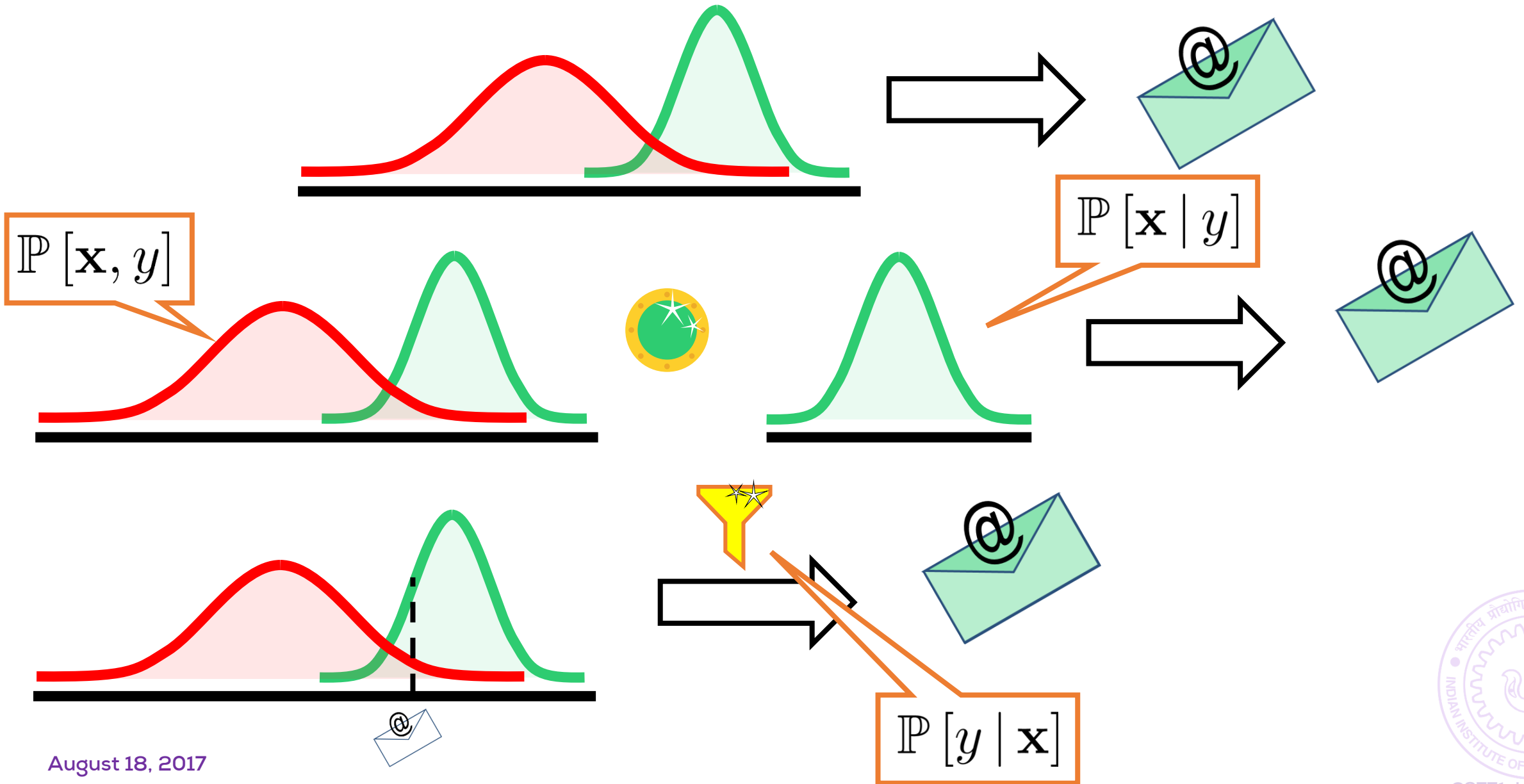
Generative Models for Labeled Data



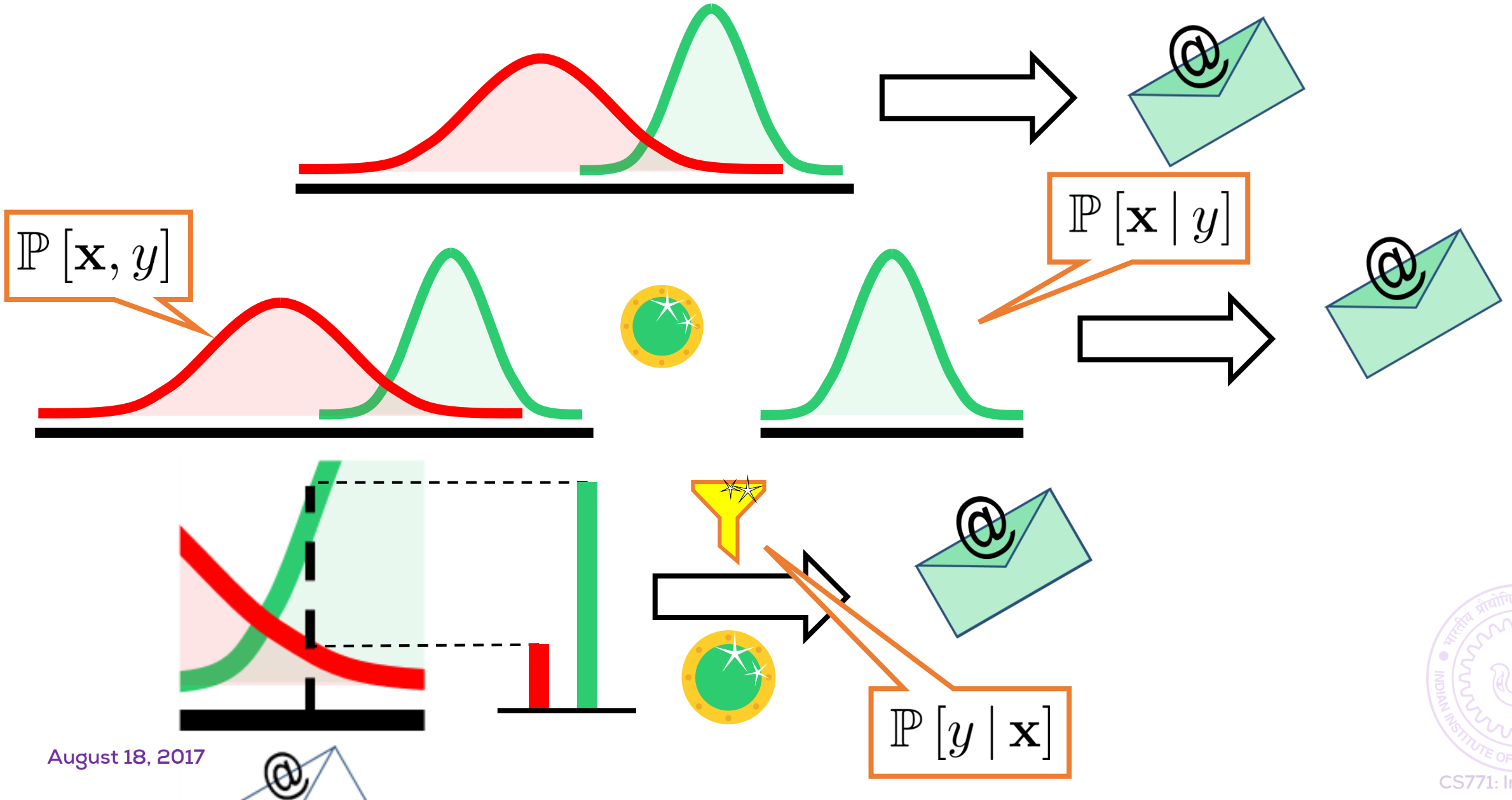
Generative Models for Labeled Data



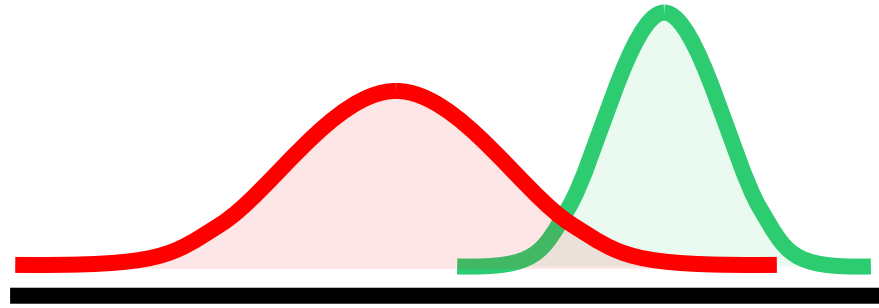
Generative Models for Labeled Data



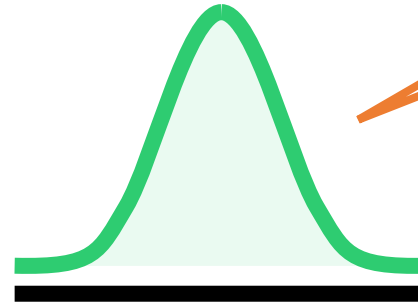
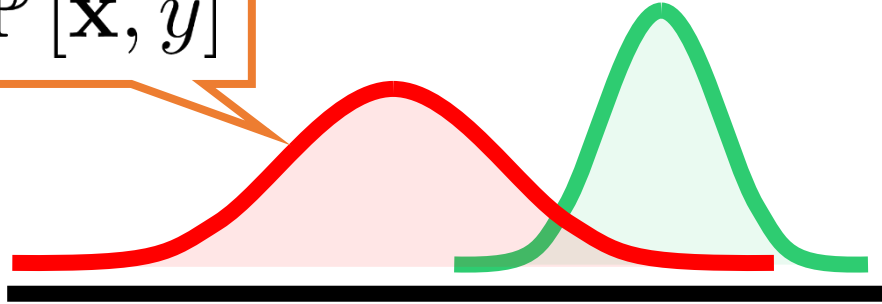
Generative Models for Labeled Data



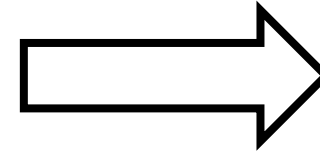
Generative Models for Labeled Data



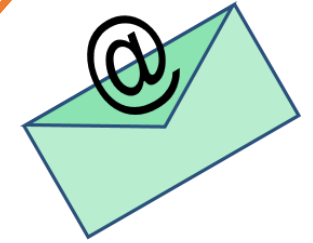
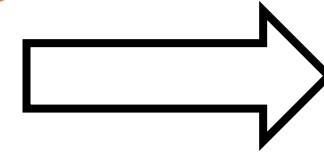
$\mathbb{P}[\mathbf{x}, y]$



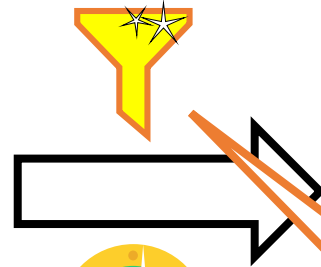
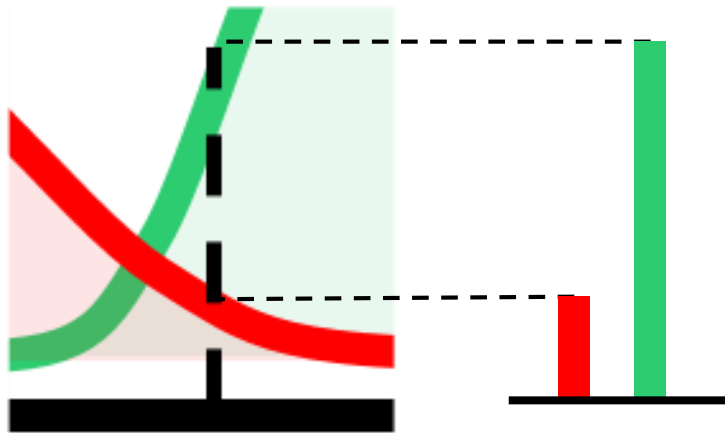
$\mathbb{P}[\mathbf{x} | y]$



Used in
generative
learning



Used in
discriminative
learning



$\mathbb{P}[y | \mathbf{x}]$

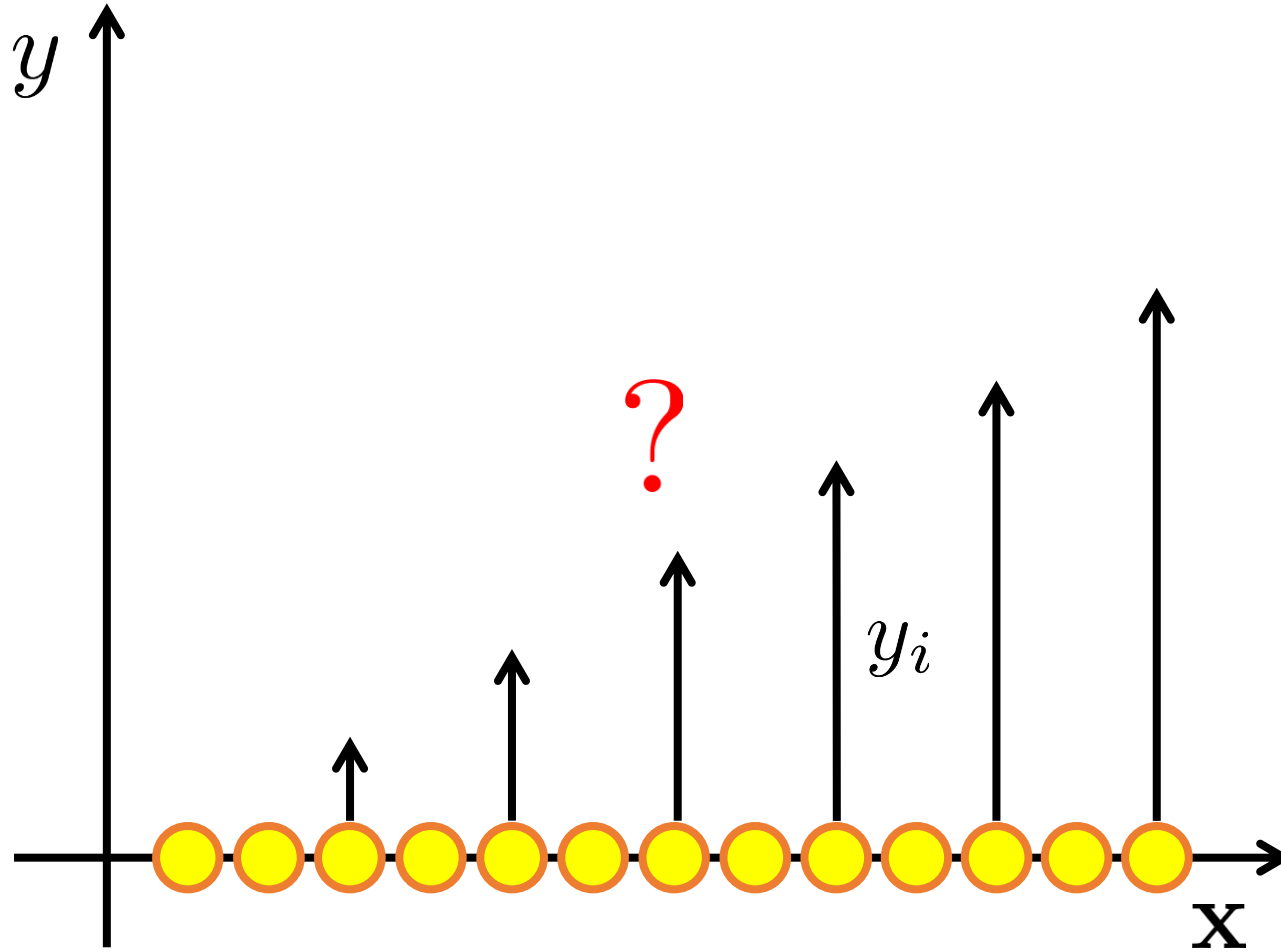


Regression using PML

August 16, 2017



Linear Regression



Data: $\mathbf{x}^1, \mathbf{x}^2, \dots, \mathbf{x}^n \in \mathbb{R}^d$

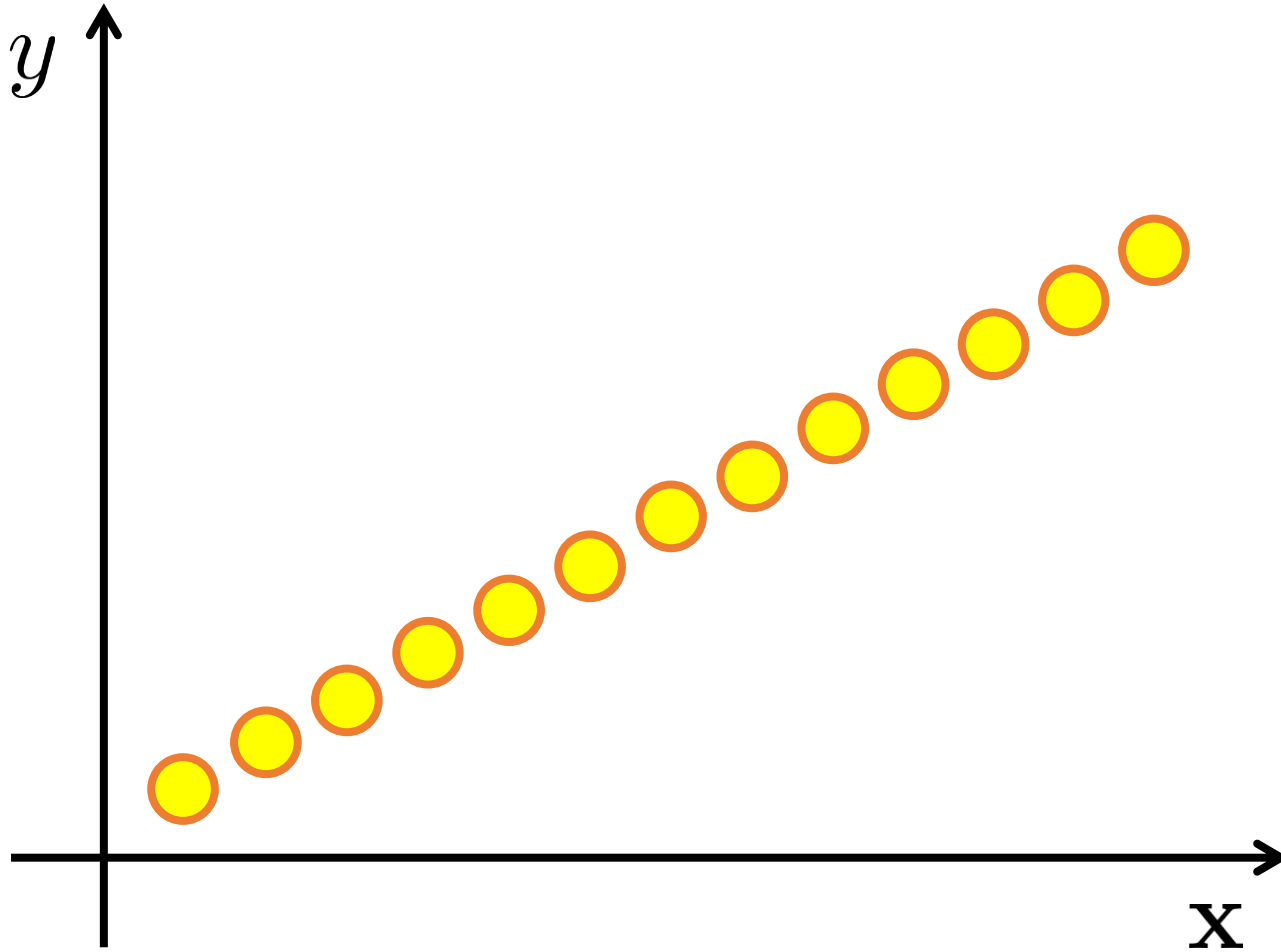
Model: \mathbf{w}^* (hidden)

$$y^i = \langle \mathbf{w}^*, \mathbf{x}^i \rangle$$

Given: $(\mathbf{x}^1, y^1), \dots, (\mathbf{x}^n, y^n)$

Recover \mathbf{w}^* ?

Linear Regression

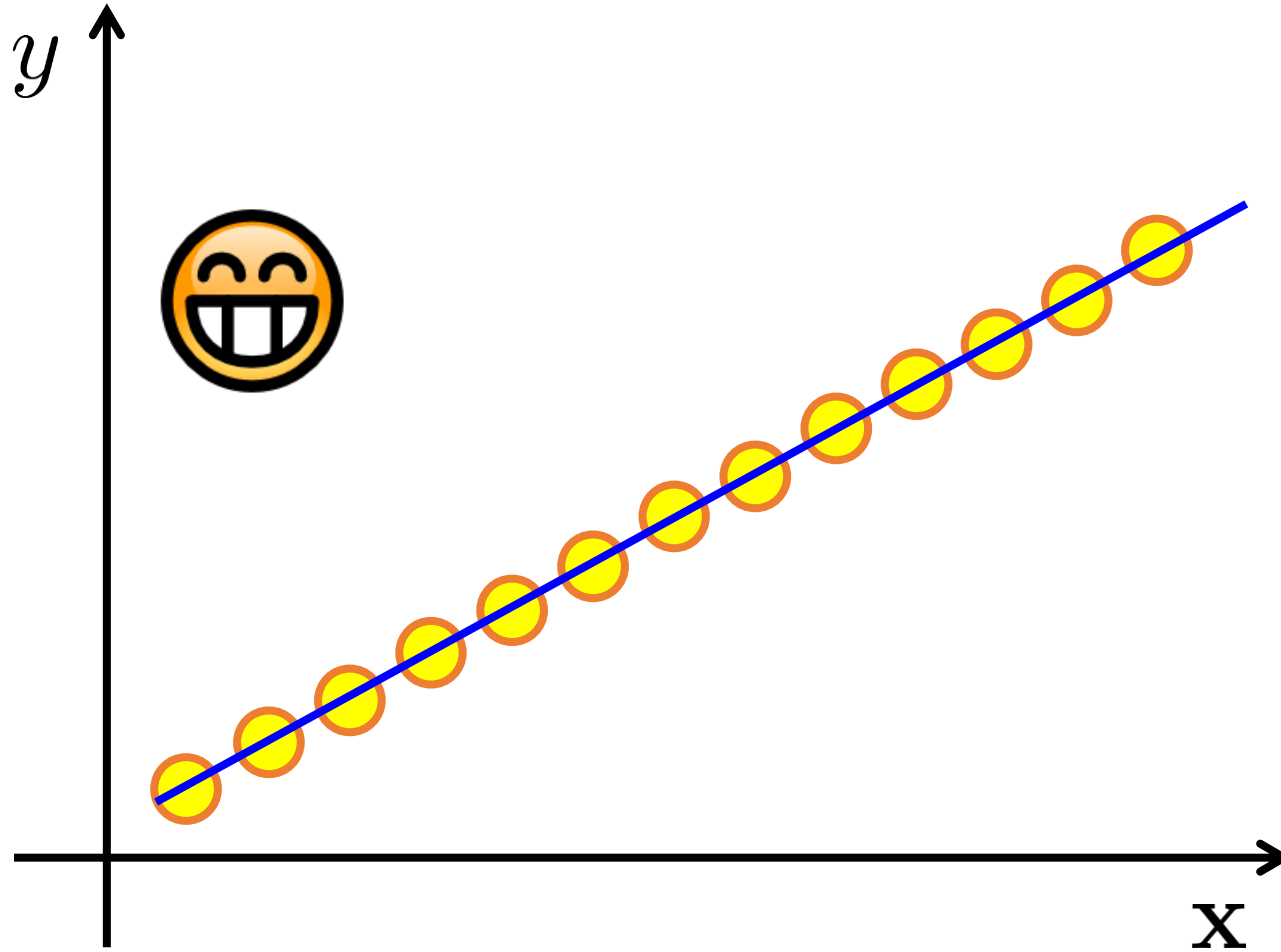


Given: $(\mathbf{x}^1, y^1), \dots, (\mathbf{x}^n, y^n)$

$$y^i = \langle \mathbf{w}^*, \mathbf{x}^i \rangle$$

$$\begin{matrix} \text{blue arrow } n \\ \left[\begin{array}{c} y^1 \\ y^2 \\ y^3 \\ \vdots \\ y^n \end{array} \right] \\ \text{blue arrow } n \\ \mathbf{y} \end{matrix} = \begin{matrix} \text{red arrow } d \\ \underbrace{\left[\begin{array}{ccc} \text{---} & \mathbf{x}^1 & \text{---} \\ \text{---} & \mathbf{x}^2 & \text{---} \\ \text{---} & \mathbf{x}^3 & \text{---} \\ & \vdots & \\ \text{---} & \mathbf{x}^n & \text{---} \end{array} \right]}_{\mathbf{X}^T} \\ \text{red arrow } d \end{matrix} \begin{matrix} \left[\begin{array}{c} | \\ \mathbf{w} \\ | \end{array} \right] \\ \text{red arrow } d \end{matrix}$$

Linear Regression



Given: $(\mathbf{x}^1, y^1), \dots, (\mathbf{x}^n, y^n)$

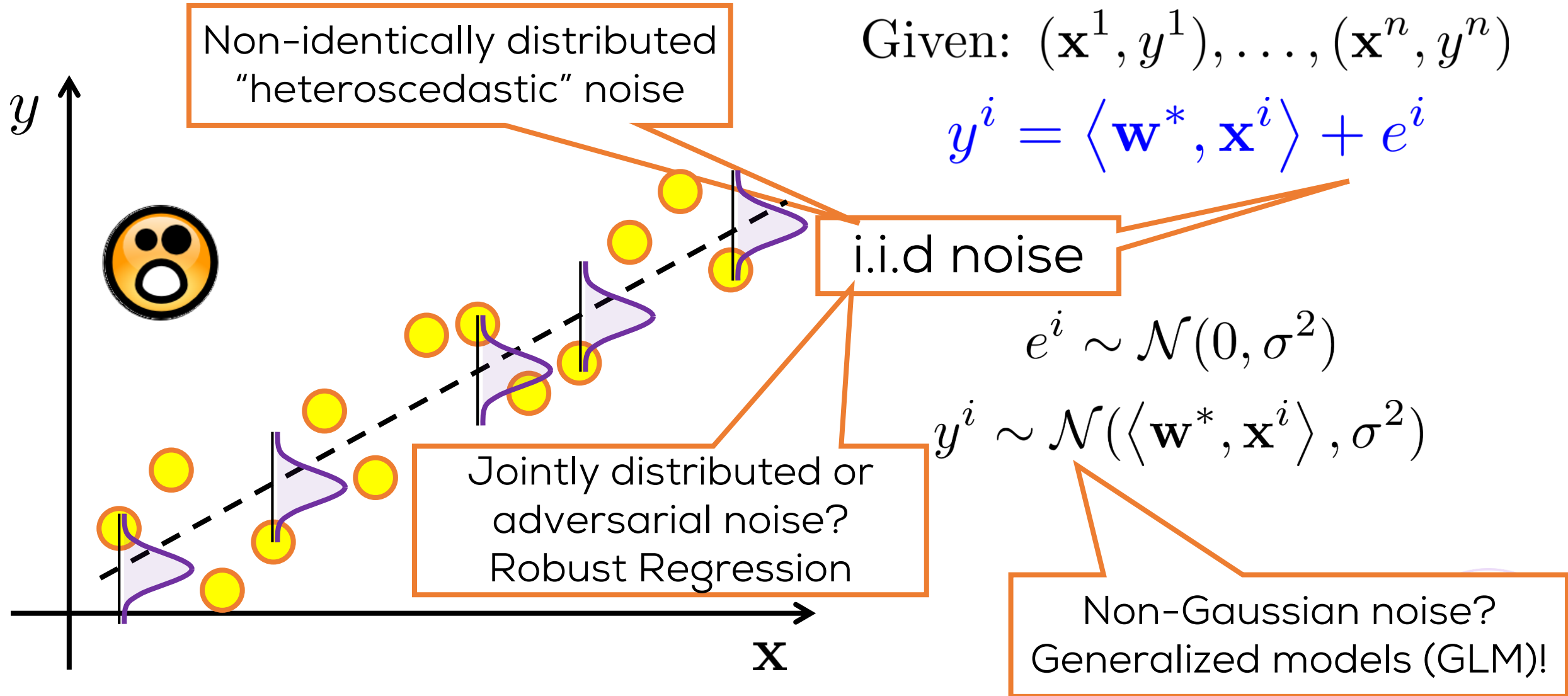
$$y^i = \langle \mathbf{w}^*, \mathbf{x}^i \rangle$$

$$\mathbf{y} = \mathbf{X}^\top \mathbf{w}$$

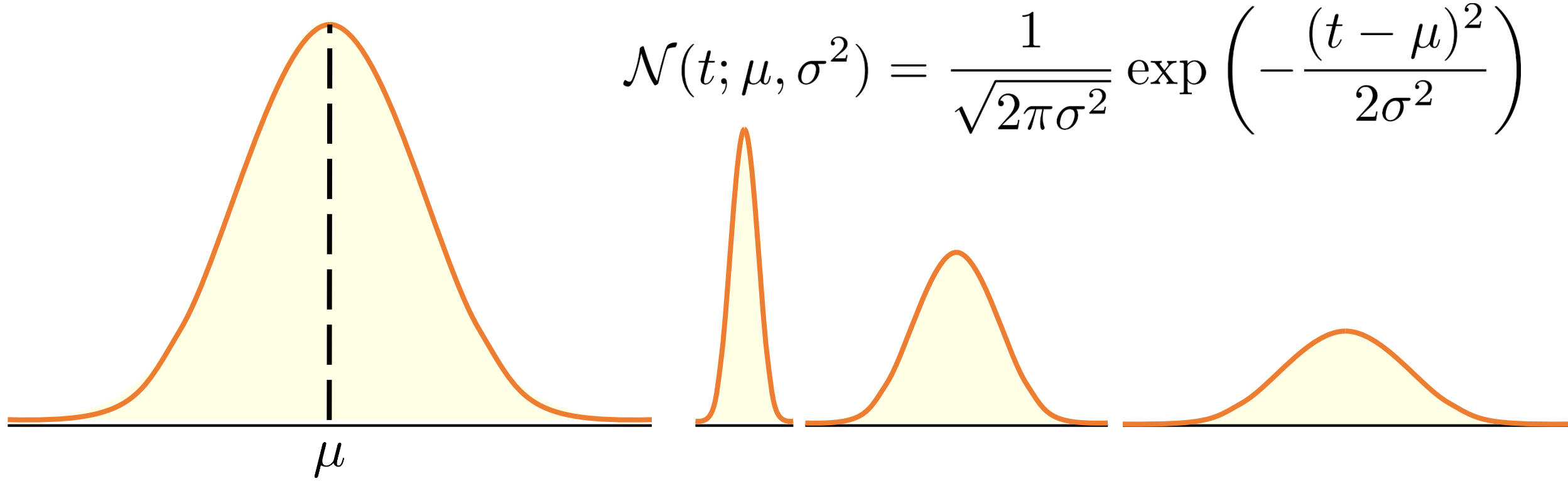
Linear system!!

\mathbf{w}^* Recovered!!

Linear Regression with Noise



The Gaussian Distribution



$$\mathcal{N}(t; \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(t - \mu)^2}{2\sigma^2}\right)$$

**Multivariate
Gaussian**

$$\mathcal{N}(\mathbf{v}; \boldsymbol{\mu}, \Sigma) = \frac{1}{\sqrt{(2\pi)^d |\Sigma|}} \exp\left(-\frac{1}{2}(\mathbf{v} - \boldsymbol{\mu})^\top \Sigma^{-1}(\mathbf{v} - \boldsymbol{\mu})\right)$$

Linear Regression using MLE

$$\mathbb{P}[y | \mathbf{x}^i, \mathbf{w}] = \mathcal{N}(\langle \mathbf{w}, \mathbf{x}^i \rangle, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y - \langle \mathbf{w}, \mathbf{x}^i \rangle)^2}{2\sigma^2}\right)$$

Linear
function

Likelihood

Why isn't \mathbf{x} getting
modelled too?

Generative
model

Log-likelihood

$$\log \mathbb{P}[\mathbf{y} | \mathbf{X}, \mathbf{w}] = C - \frac{1}{2\sigma^2} \sum_{i=1}^n (y^i - \langle \mathbf{w}, \mathbf{x}^i \rangle)^2$$

Least Squares!

$$\hat{\mathbf{w}}_{\text{MLE}} = \arg \min \sum_{i=1}^n (y^i - \langle \mathbf{w}, \mathbf{x}^i \rangle)^2 = (\mathbf{X}\mathbf{X}^\top)^\dagger \mathbf{X}\mathbf{y}$$

$\log \mathbb{P}[\mathbf{y}, \mathbf{X} | \boldsymbol{\theta}]$
Generative
MLE??

Exercise

Linear Regression using MAP

$$\mathbb{P}[\mathbf{w}] = \mathcal{N}(\mathbf{0}, \rho^2 \cdot I_d) = \frac{1}{\sqrt{(2\pi\rho^2)^d}} \exp\left(-\frac{\|\mathbf{w}\|_2^2}{2\rho^2}\right)$$

Can use sparsity
inducing priors too!

$$\log \mathbb{P}[\mathbf{w} | \mathbf{X}, \mathbf{y}] = C - \frac{1}{2\sigma^2} \sum_{i=1}^n (y^i - \langle \mathbf{w}, \mathbf{x}^i \rangle)^2 - \frac{1}{2\rho^2} \|\mathbf{w}\|_2^2$$

$$\hat{\mathbf{w}}_{\text{MAP}} = \arg \min \sum_{i=1}^n (y^i - \langle \mathbf{w}, \mathbf{x}^i \rangle)^2 + \frac{\sigma^2}{\rho^2} \|\mathbf{w}\|_2^2 = (\mathbf{X}\mathbf{X}^\top + \lambda I)^{-1} \mathbf{X}\mathbf{y}$$

Ridge Regression

Exercise

$\log \mathbb{P}[\boldsymbol{\theta} | \mathbf{y}, \mathbf{X}]$
Generative
MAP??

Bayesian Linear Regression?

$$\mathbb{P}[\mathbf{w} \mid \mathbf{X}, \mathbf{y}] = \mathcal{N}(\boldsymbol{\nu}, \Lambda)$$

Cool! Posterior is Gaussian like the prior!

$$\boldsymbol{\nu} = \left(\mathbf{X}\mathbf{X}^\top + \frac{\sigma^2}{\rho^2} \cdot I \right)^{-1} \mathbf{X}\mathbf{y}$$
$$\Lambda = \left(\frac{1}{\sigma^2} \mathbf{X}\mathbf{X}^\top + \frac{1}{\rho^2} \cdot I \right)^{-1}$$

Wait! MAP?

By definition, MAP is the mode of the posterior

$$\mathbb{P}[y \mid \mathbf{x}, \mathbf{X}, \mathbf{y}] = \int_{\mathbf{w}} \mathbb{P}[y \mid \mathbf{x}, \mathbf{w}] \mathbb{P}[\mathbf{w} \mid \mathbf{X}, \mathbf{y}] d\mathbf{w}$$
$$= \mathcal{N}(\langle \boldsymbol{\nu}, \mathbf{x} \rangle, \sigma^2 + \mathbf{x}^\top \Lambda \mathbf{x})$$

Predictive Posterior

Extra Information

A few Thoughts

- Do I have to use these very forms for likelihood and prior?

$$\mathbb{P} [y \mid \mathbf{x}^i, \boldsymbol{\theta}] = \mathcal{D}(\langle \mathbf{w}, \mathbf{x}^i \rangle)$$

- No, however some choices make sense and make estimation easier
- Conjugacy makes life very simple if possible to achieve
- Look at your application and take these decisions
 - If you know your model is sparse, use a Laplacian prior
 - If you know your noise is not Gaussian, use a GLM
- Can I build probabilistic models for other ML tasks as well?
 - Yes, of course. We will look at classification problems next.
 - We can do probabilistic clustering, dim. redn., ranking
 - There are entire courses devoted to PML techniques: CS772, CS698S

A few Thoughts

- What about non-linear regression?

$$\mathbb{P} [y \mid \mathbf{x}^i, \boldsymbol{\theta}] = \mathcal{N}(f(\mathbf{x}^i, \boldsymbol{\theta}), \sigma^2)$$

- MLE, MAP estimation more challenging - kernel methods, deep learning
- Gaussian processes more suited for non-linear PML – beyond the scope!
- Are Bayesian models better than non-Bayesian ones?
 - Bayesian models more informative $\mathcal{N}(\langle \boldsymbol{\nu}, \mathbf{x} \rangle, \sigma^2 + \mathbf{x}^\top \Lambda \mathbf{x})$
 - Useful in settings like active learning, anomaly detection
 - Can be more expensive at training and prediction time
 - Ask your doctor if your application needs Bayesian reasoning or not!
- Bayesian \neq Generative

A few Thoughts

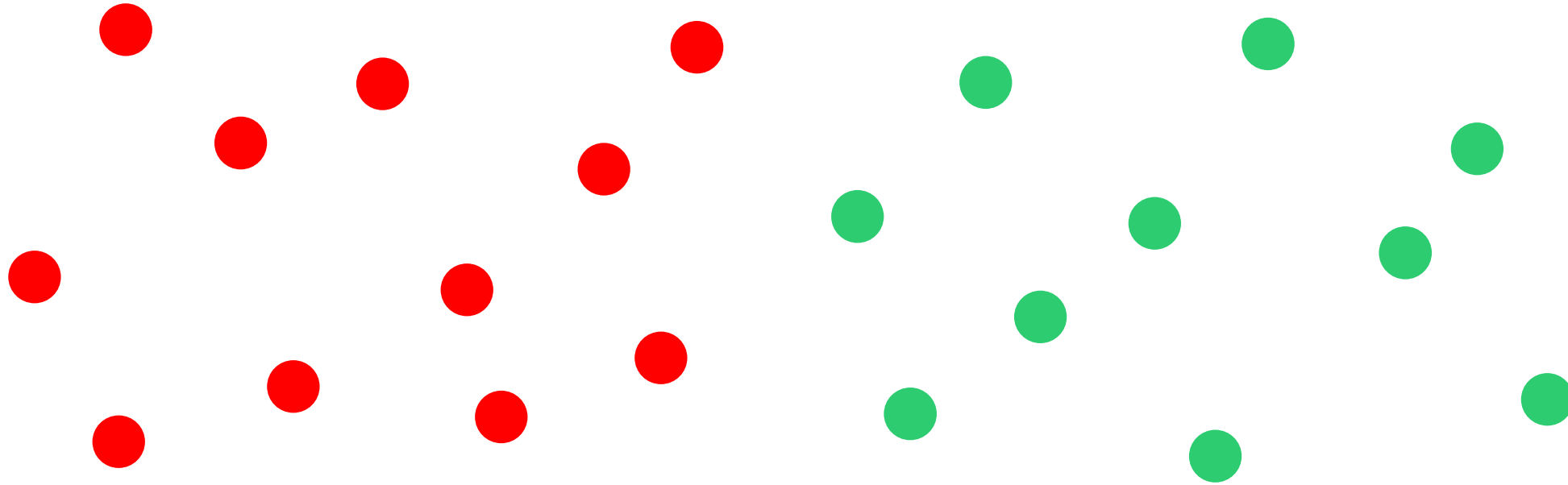
- How do I solve all these optimization problems that MLE, MAP procedures keep throwing up?
 - We are in safe hands – optimization theory is very evolved
 - Wait for the next set of lectures on function approximation methods
- Are generatively trained models better or discriminative ones?
 - Discriminative models reason about $\mathbb{P}[y|\mathbf{x}]$
 - Generative models reason about $\mathbb{P}[y, \mathbf{x}]$
 - For prediction, all we need is $\mathbb{P}[y|\mathbf{x}]$
 - Generative models handle missing, erroneous data easily but bulky
 - Discriminative models are much lighter, easier to train
 - Models such GMMs, deep nets, can be trained in gen. and disc. manner

Classification using PML

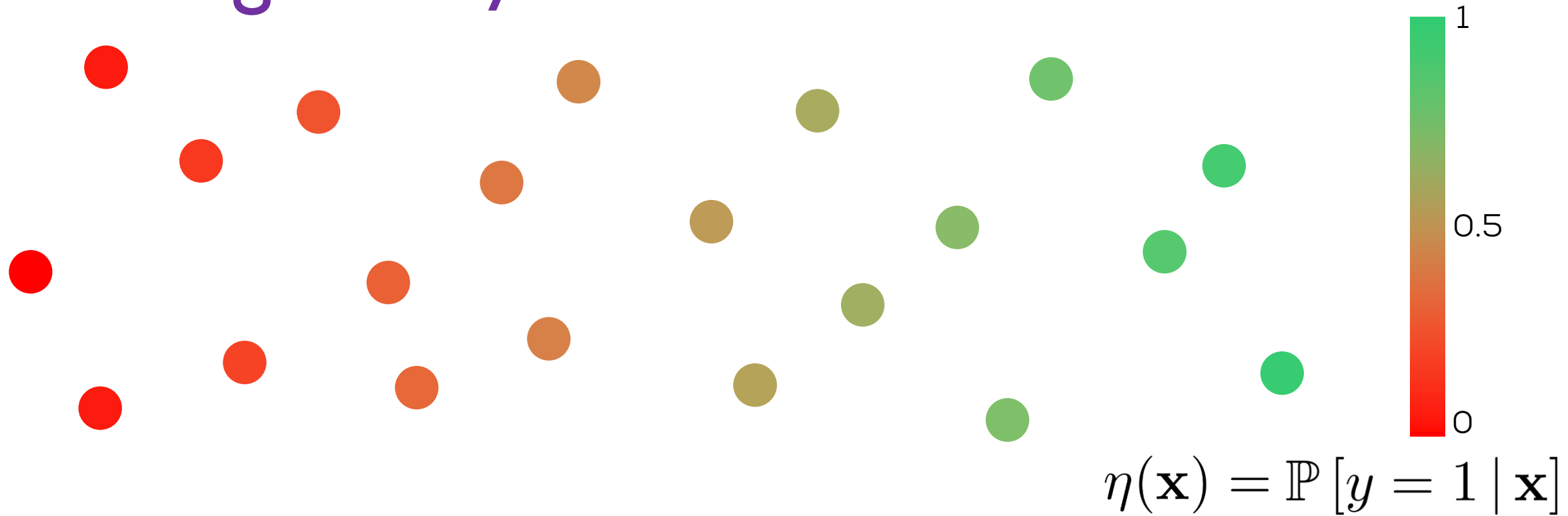
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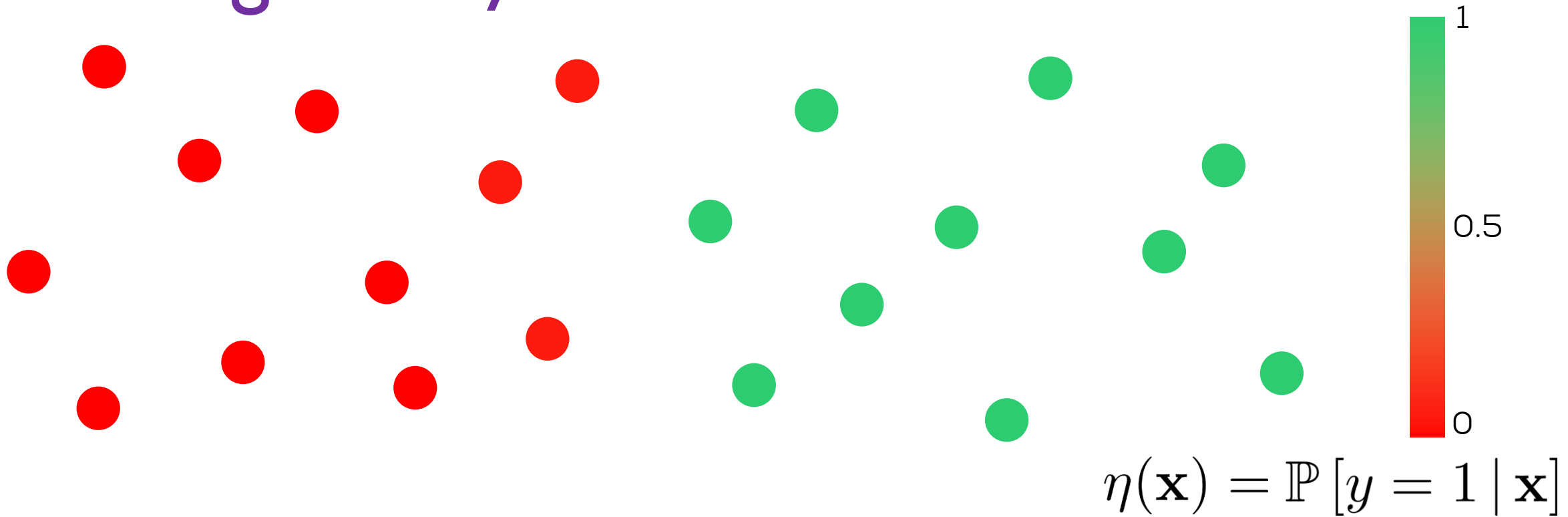
Revisiting Binary Classification



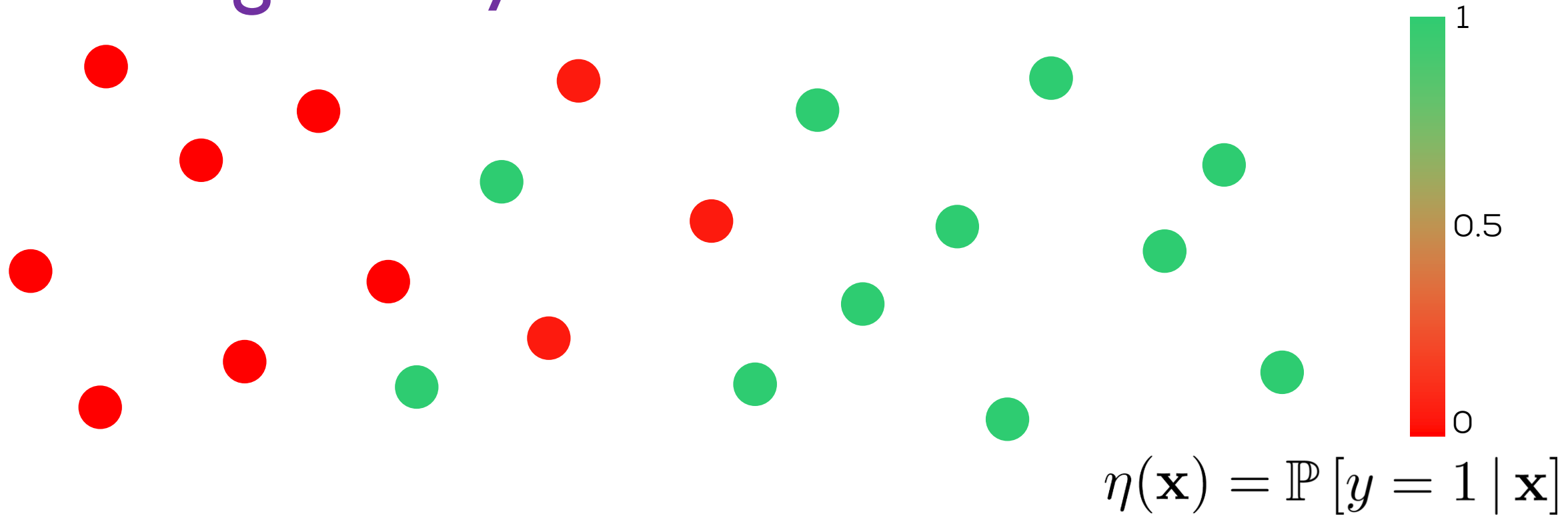
Revisiting Binary Classification



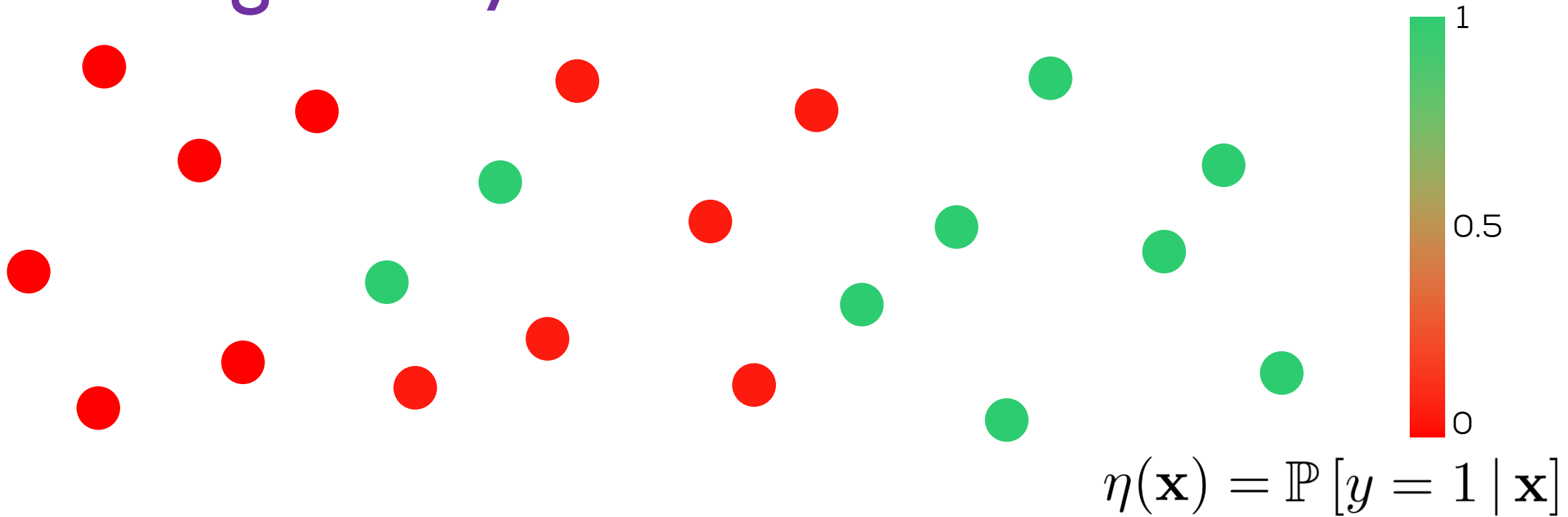
Revisiting Binary Classification



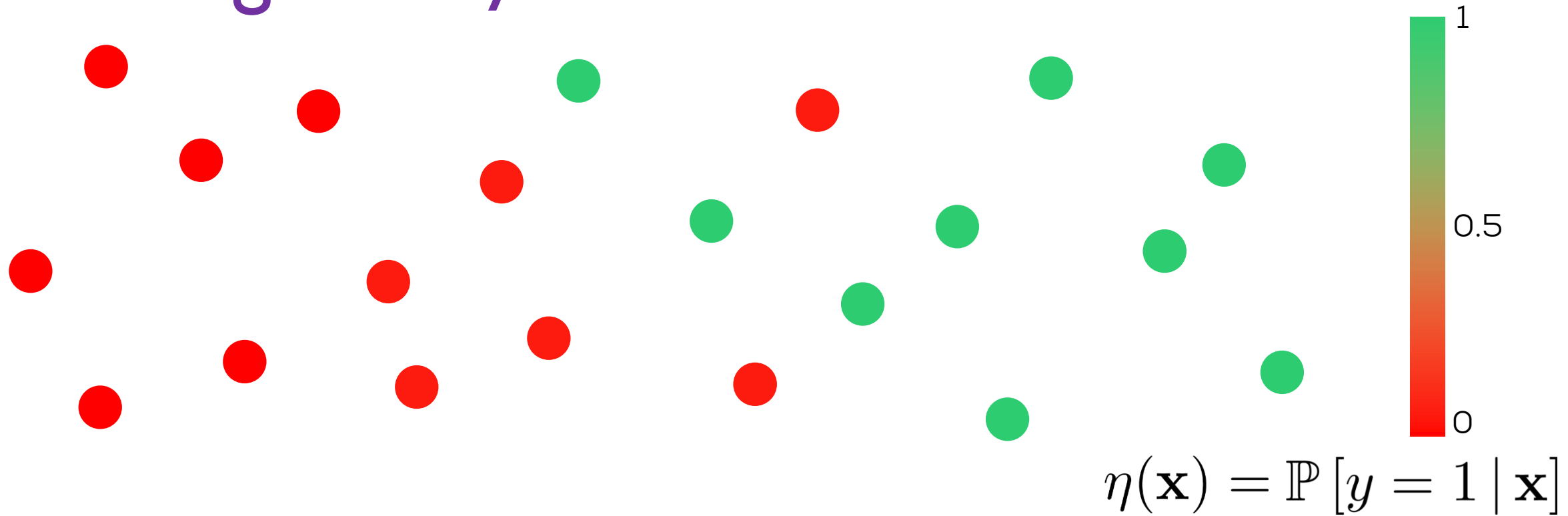
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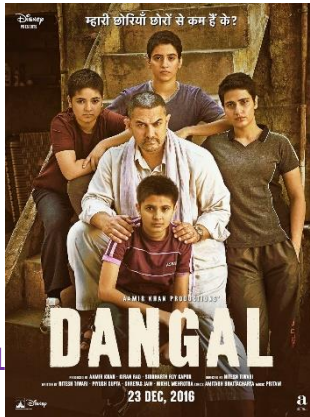
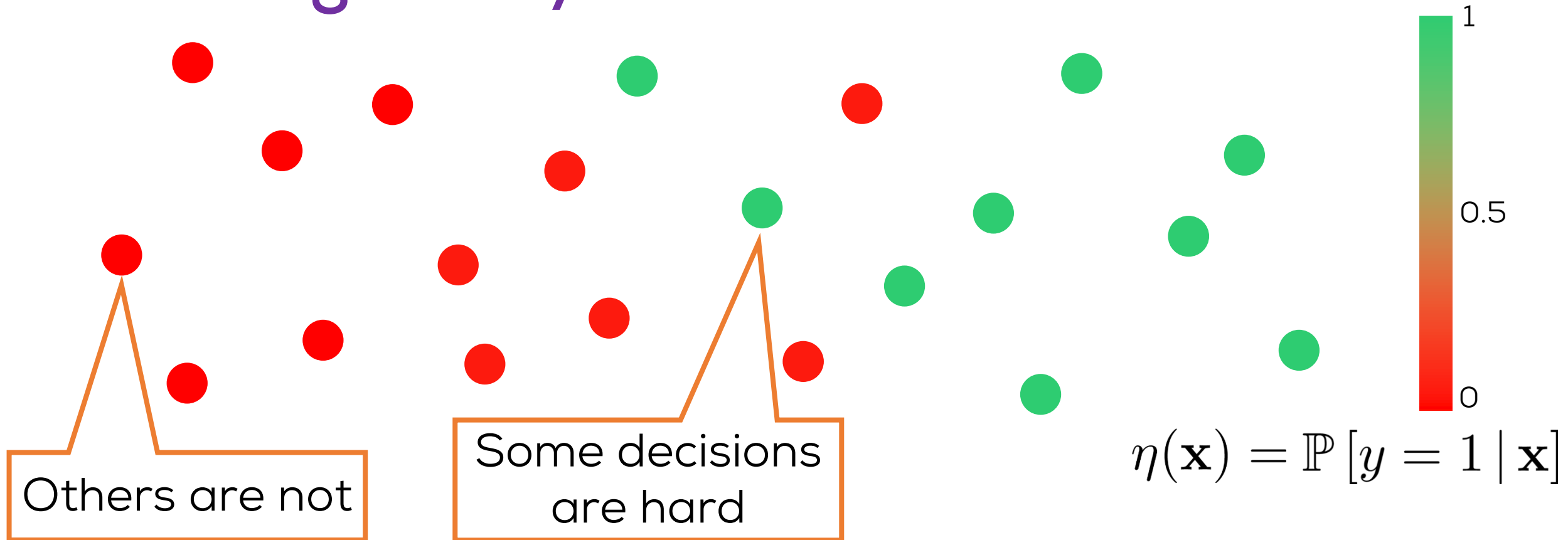
Revisiting Binary Classification



Revisiting Binary Classification



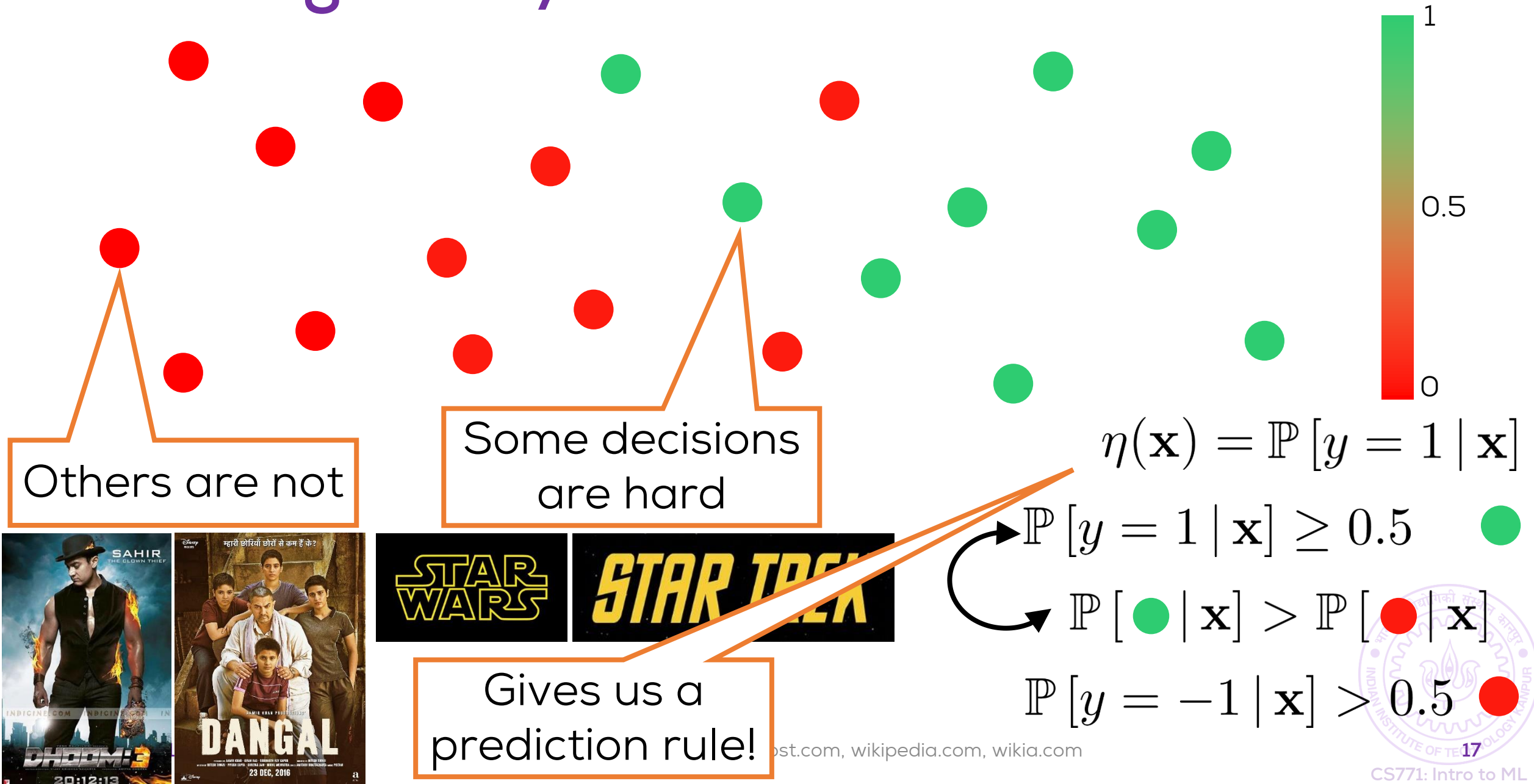
Revisiting Binary Classification



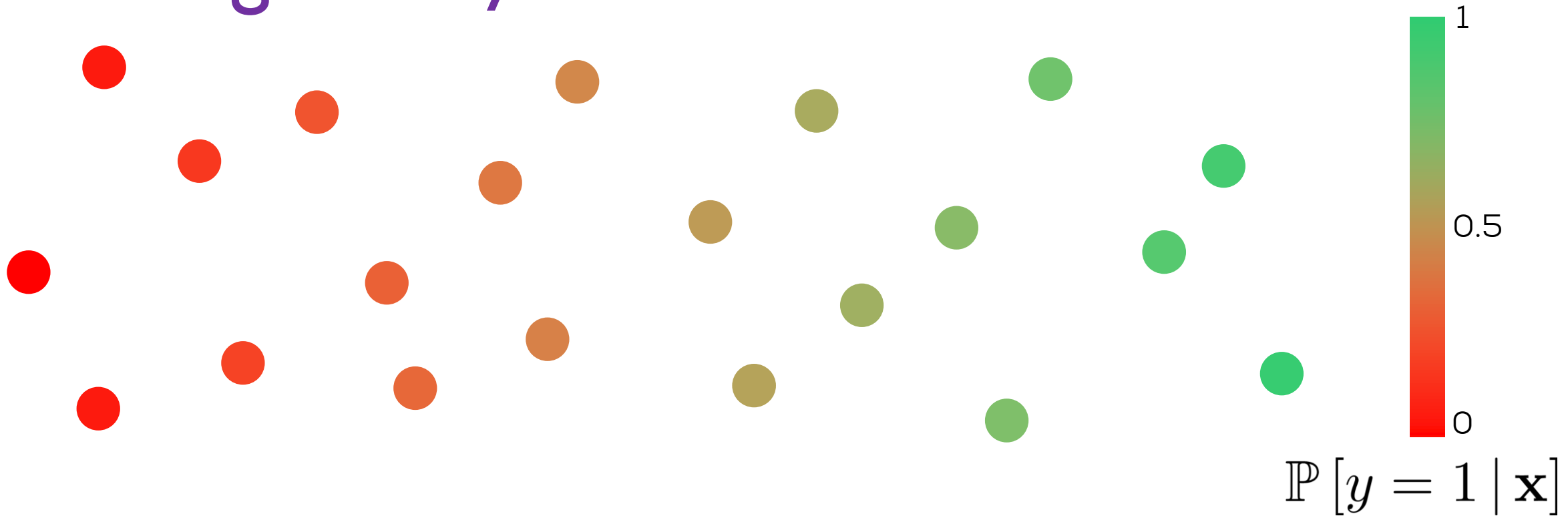
subscene.com, firstpost.com, wikipedia.com, wikia.com



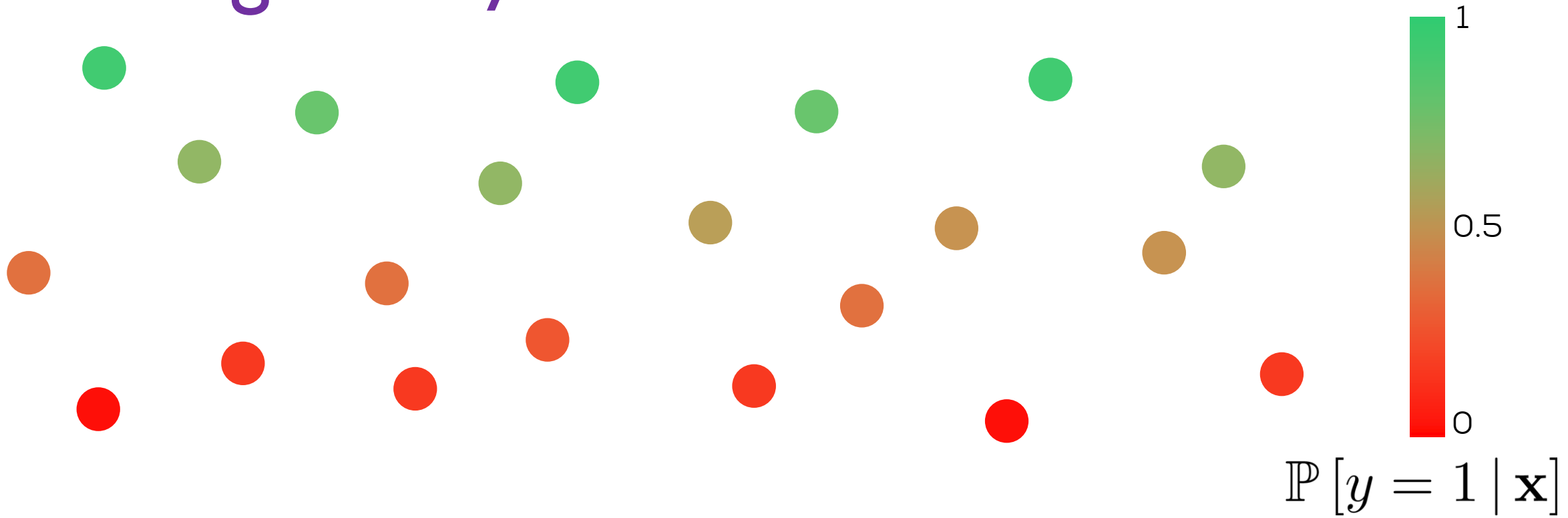
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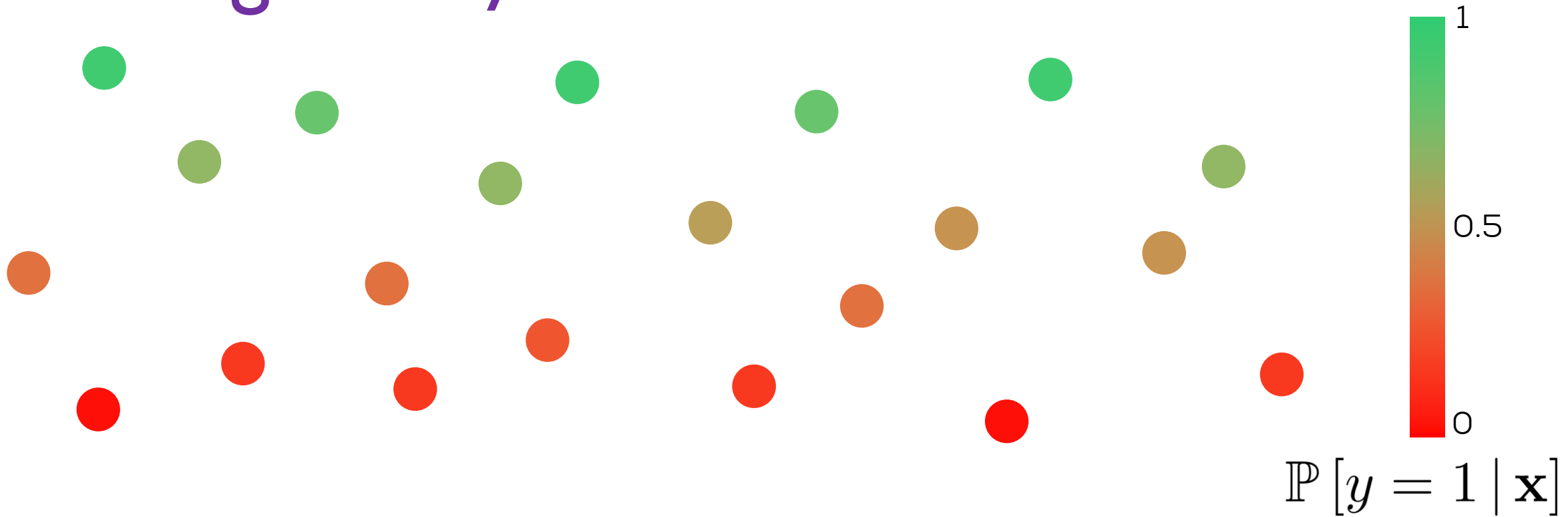
Revisiting Binary Classification



Revisiting Binary Classification

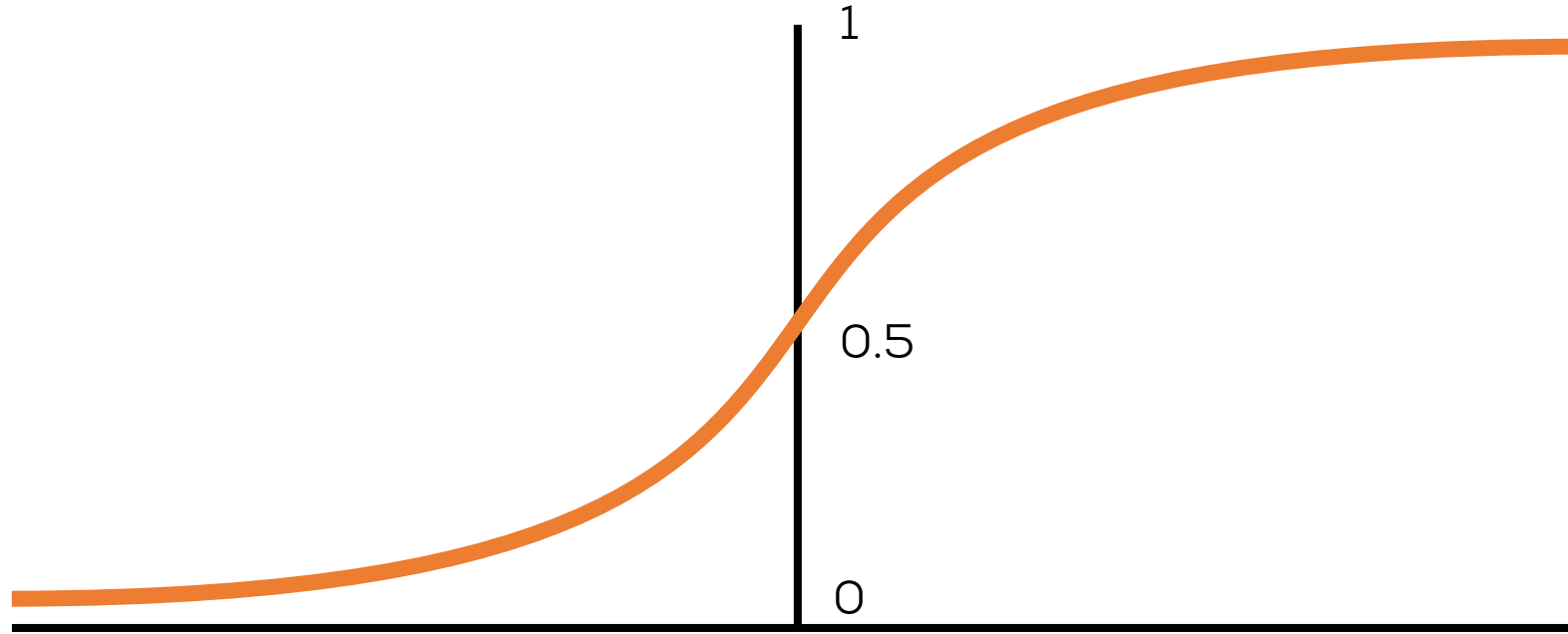


Revisiting Binary Classification



Features Matter!

The Sigmoid Function



$$\sigma(t) = \frac{1}{1 + \exp(-t)} = \frac{\exp(t)}{\exp(t) + 1}$$

Classification using MLE

$$\mathbb{P}[y | \mathbf{x}^i, \mathbf{w}] = \sigma(y \langle \mathbf{w}, \mathbf{x}^i \rangle) = \frac{1}{1 + \exp(-y \langle \mathbf{w}, \mathbf{x}^i \rangle)}$$

Shorthand
 $\mathbb{P}[y^i = y] =: \mathbb{P}[y]$

$$\mathbb{P}[y^i = 1 | \mathbf{x}^i, \mathbf{w}] + \mathbb{P}[y^i = -1 | \mathbf{x}^i, \mathbf{w}] = 1$$

Likelihood

$$\log \frac{\mathbb{P}[y^i = 1 | \mathbf{x}^i, \mathbf{w}]}{\mathbb{P}[y^i = -1 | \mathbf{x}^i, \mathbf{w}]} = \langle \mathbf{w}, \mathbf{x}^i \rangle$$

Log-odds

Log-likelihood

$$\log \mathbb{P}[\mathbf{y} | \mathbf{X}, \mathbf{w}] = \sum_{i=1}^n \log \left(\frac{1}{1 + \exp(-y^i \langle \mathbf{w}, \mathbf{x}^i \rangle)} \right)$$

$\hat{\mathbf{w}}_{\text{MLE}} = ?$

Wait for learning
with FA

$$f(t) = -\log(\sigma(t))$$

Another possibility

- What happens if $y_i \in \{0,1\}$ instead of $y_i \in \{-1,1\}$?
- Binomial instead of Rademacher
- How to redefine likelihood?
- Need to ensure $\mathbb{P}[y^i = 1 \mid \mathbf{x}^i, \mathbf{w}] + \mathbb{P}[y^i = 0 \mid \mathbf{x}^i, \mathbf{w}] = 1$
- One way is the following

$$\hat{\eta}_i = \sigma(\langle \mathbf{w}, \mathbf{x}^i \rangle)$$

$$\mathbb{P}[y^i \mid \mathbf{x}^i, \mathbf{w}] = (\hat{\eta}_i)^{y^i} \cdot (1 - \hat{\eta}_i)^{1-y^i}$$

- Do you get the same MLE problem?
- What about MAP estimates? $\mathbb{P}[\mathbf{w}] = \mathcal{N}(\mathbf{0}, \rho^2 \cdot I_d)$

Bayesian Logistic Regression?



$$\mathbb{P}[y \mid \mathbf{x}, \mathbf{w}] = \sigma(y \langle \mathbf{w}, \mathbf{x} \rangle)$$

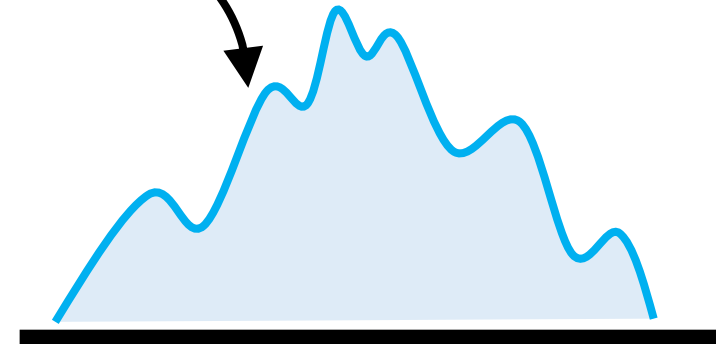
$$\mathbb{P}[\mathbf{w}] = \mathcal{N}(\mathbf{0}, \rho^2 \cdot I_d)$$

$$\mathbb{P}[\mathbf{w} \mid \mathbf{X}, \mathbf{y}] = \frac{\mathbb{P}[\mathbf{y} \mid \mathbf{X}, \mathbf{w}] \mathbb{P}[\mathbf{w}]}{\int_{\mathbf{w}'} \mathbb{P}[\mathbf{y} \mid \mathbf{X}, \mathbf{w}'] \mathbb{P}[\mathbf{w}'] d\mathbf{w}'} = \frac{\prod_{i=1}^n \sigma(y^i \langle \mathbf{w}, \mathbf{x}^i \rangle)}{\int_{\mathbf{w}'} \prod_{i=1}^n \sigma(y^i \langle \mathbf{w}', \mathbf{x}^i \rangle) \exp\left(-\frac{\|\mathbf{w}'\|_2^2}{2\sigma^2}\right) d\mathbf{w}'}$$

Posterior Approximation

MCMC, Variational Inference,
Laplace approx

$\mathbb{P}[\mathbf{w} \mid \mathbf{X}, \mathbf{y}]$



Bayesian Logistic Regression?



$$\mathbb{P}[y | \mathbf{x}, \mathbf{w}] = \sigma(y \langle \mathbf{w}, \mathbf{x} \rangle)$$

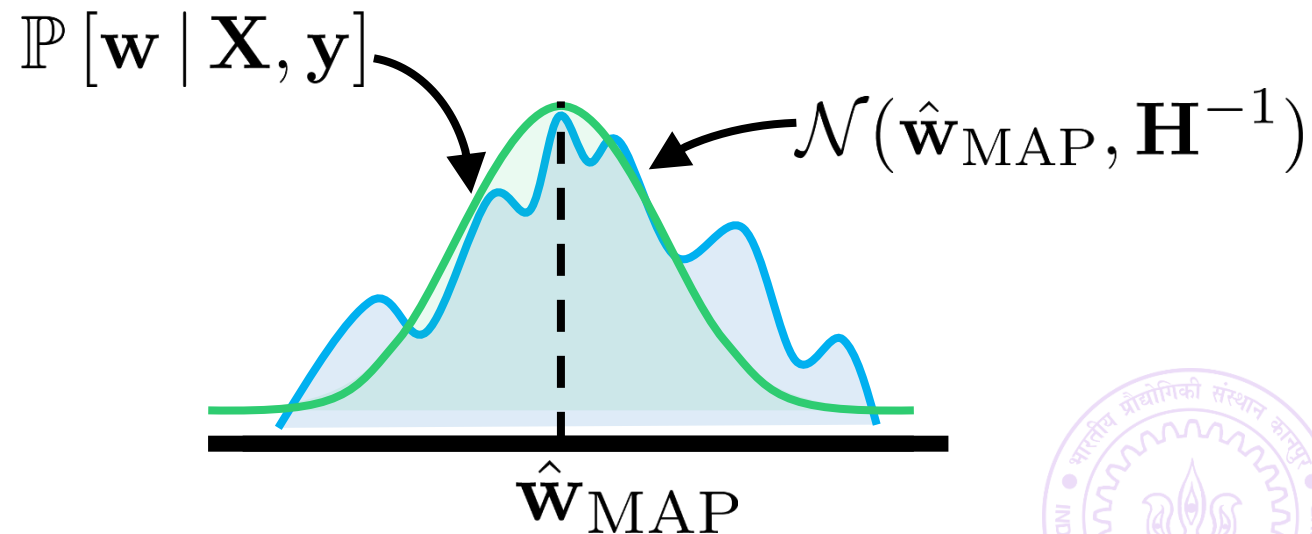
$$\mathbb{P}[\mathbf{w}] = \mathcal{N}(\mathbf{0}, \rho^2 \cdot I_d)$$

$$\mathbb{P}[\mathbf{w} | \mathbf{X}, \mathbf{y}] = \frac{\mathbb{P}[\mathbf{y} | \mathbf{X}, \mathbf{w}] \mathbb{P}[\mathbf{w}]}{\int_{\mathbf{w}'} \mathbb{P}[\mathbf{y} | \mathbf{X}, \mathbf{w}'] \mathbb{P}[\mathbf{w}'] d\mathbf{w}'} = \frac{\prod_{i=1}^n \sigma(y^i \langle \mathbf{w}, \mathbf{x}^i \rangle)}{\int_{\mathbf{w}'} \prod_{i=1}^n \sigma(y^i \langle \mathbf{w}', \mathbf{x}^i \rangle) \exp\left(-\frac{\|\mathbf{w}'\|_2^2}{2\sigma^2}\right) d\mathbf{w}'}$$

Posterior Approximation

MCMC, Variational Inference,
Laplace approx

However, even the Laplace predictive posterior is intractable ☹



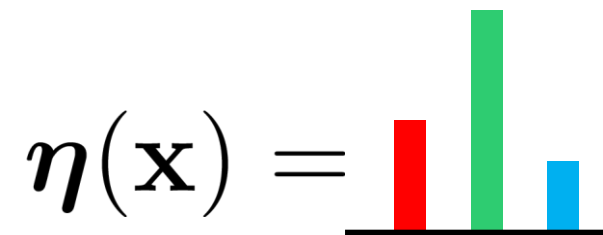
Multi-class and Multi-label Classification using PML

August 16, 2017



Multi-classification using MLE

- $K > 2$ classes – need more detailed parameters
- For each point, its label profile is a vector



$$\mathbb{P} [y^i = k \mid \mathbf{x}^i, \{\mathbf{w}^l\}_{1,\dots,K}] \propto \exp(\langle \mathbf{w}^k, \mathbf{x}^i \rangle)$$

$$\mathbb{P} [y^i = k \mid \mathbf{x}^i, \{\mathbf{w}^l\}_{1,\dots,K}] = \frac{\exp(\langle \mathbf{w}^k, \mathbf{x}^i \rangle)}{\sum_{l=1}^K \exp(\langle \mathbf{w}^l, \mathbf{x}^i \rangle)}$$

- Likelihood function is multinomial instead of binomial

$$\mathbb{P} [\mathbf{y} \mid \mathbf{X}, \mathbf{w}] = \prod_{i=1}^n \hat{\eta}_{y^i}^i(\mathbf{x}) \quad \hat{\eta}_k^i(\mathbf{x}) = \frac{\exp(\langle \mathbf{w}^k, \mathbf{x}^i \rangle)}{\sum_{l=1}^K \exp(\langle \mathbf{w}^l, \mathbf{x}^i \rangle)}$$

Softmax Regression

Binary vs Multi-Classification using Linear LR

- Binary

$$\arg \max_{y \in \{-1, 1\}} \mathbb{P}[y \mid \mathbf{x}]$$

- Multiclass



Binary vs Multi-Classification using Linear LR

- Binary

$$\mathbb{P}[y \mid \mathbf{x}] \geq 0.5$$

- Multiclass



Binary vs Multi-Classification using Linear LR

- Binary

$$\mathbb{P}[y \mid \mathbf{x}] \geq 0.5$$

$$\mathbb{P}[y \mid \mathbf{x}, \mathbf{w}] = \sigma(y \langle \mathbf{w}, \mathbf{x} \rangle)$$

- Multiclass



Binary vs Multi-Classification using Linear LR

- Binary

$$\sigma(y \langle \mathbf{w}, \mathbf{x}^i \rangle) \geq 0.5$$

- Multiclass



Binary vs Multi-Classification using Linear LR

- Binary

$$y \langle \mathbf{w}, \mathbf{x}^i \rangle \geq 0$$

- Multiclass



Binary vs Multi-Classification using Linear LR

- Binary

$$y = \text{sign}(\langle \mathbf{w}, \mathbf{x}^i \rangle)$$

- Multiclass



Binary vs Multi-Classification using Linear LR

- Binary

$$y = \text{sign}(\langle \mathbf{w}, \mathbf{x}^i \rangle)$$

- Multiclass

Binary vs Multi-Classification using Linear LR

- Binary

$$y = \text{sign}(\langle \mathbf{w}, \mathbf{x}^i \rangle)$$

- Multiclass

$$\arg \max_{y \in [K]} \mathbb{P}[y | \mathbf{x}]$$

Binary vs Multi-Classification using Linear LR

- Binary

$$y = \text{sign}(\langle \mathbf{w}, \mathbf{x}^i \rangle)$$

- Multiclass

$$\arg \max_{y \in [K]} \mathbb{P}[y | \mathbf{x}]$$

$$\mathbb{P}[y = k | \mathbf{x}, \mathbf{w}] = \sigma(\langle \mathbf{w}^k, \mathbf{x} \rangle)$$

Binary vs Multi-Classification using Linear LR

- Binary

$$y = \text{sign}(\langle \mathbf{w}, \mathbf{x}^i \rangle)$$

- Multiclass

$$\arg \max_{y \in [K]} \sigma(\langle \mathbf{w}^k, \mathbf{x} \rangle)$$

Binary vs Multi-Classification using Linear LR

- Binary

$$y = \text{sign}(\langle \mathbf{w}, \mathbf{x}^i \rangle)$$

- Multiclass

$$\arg \max_{y \in [K]} \langle \mathbf{w}^k, \mathbf{x} \rangle$$

Binary vs Multi-Classification using Linear LR

- Binary

$$y = \text{sign}(\langle \mathbf{w}, \mathbf{x}^i \rangle)$$

- Multiclass

$$\arg \max_{y \in [K]} \langle \mathbf{w}^k, \mathbf{x} \rangle$$

Binary vs Multi-Classification using Linear LR

- Binary

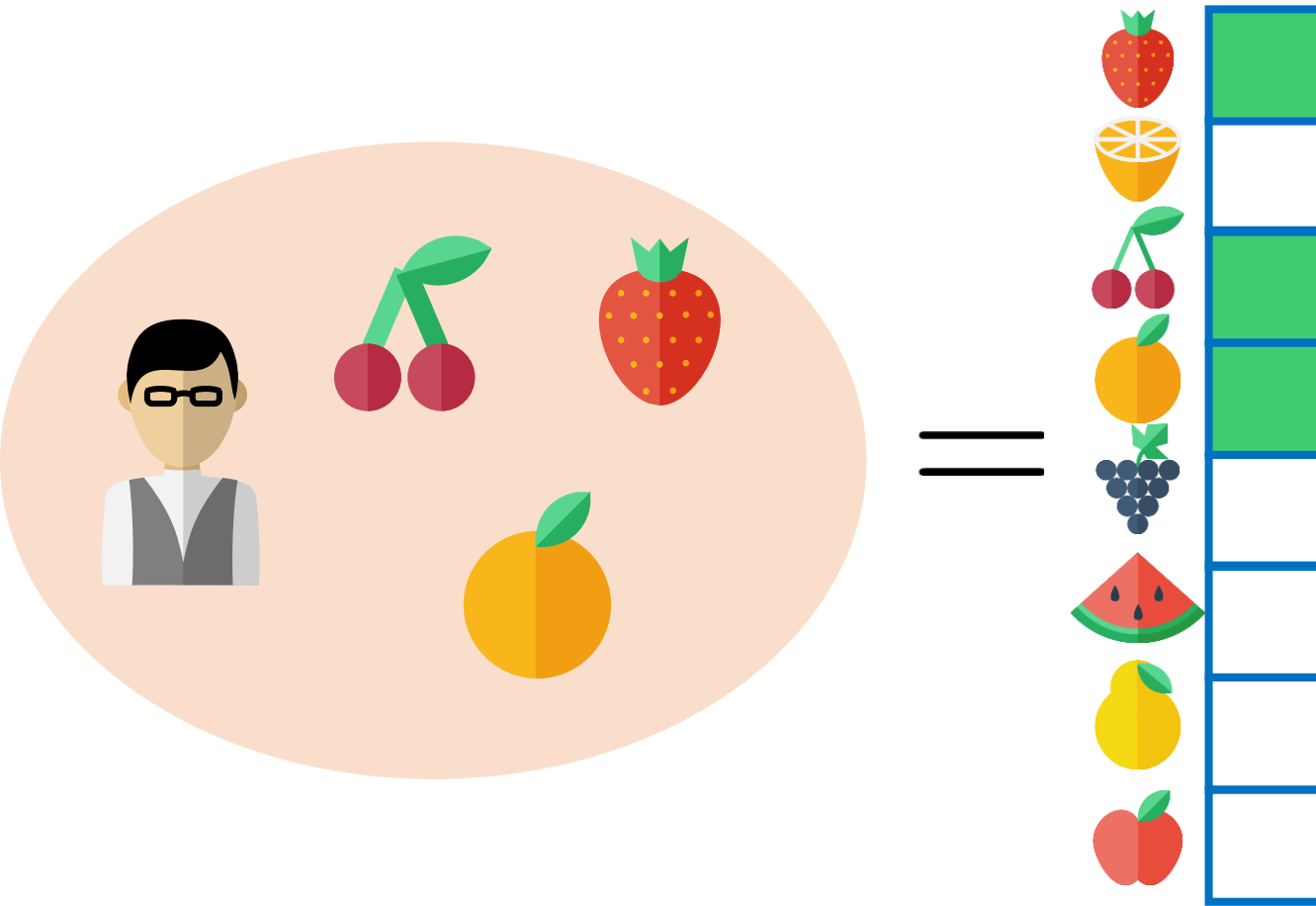
$$y = \text{sign}(\langle \mathbf{w}, \mathbf{x}^i \rangle)$$

- Multiclass

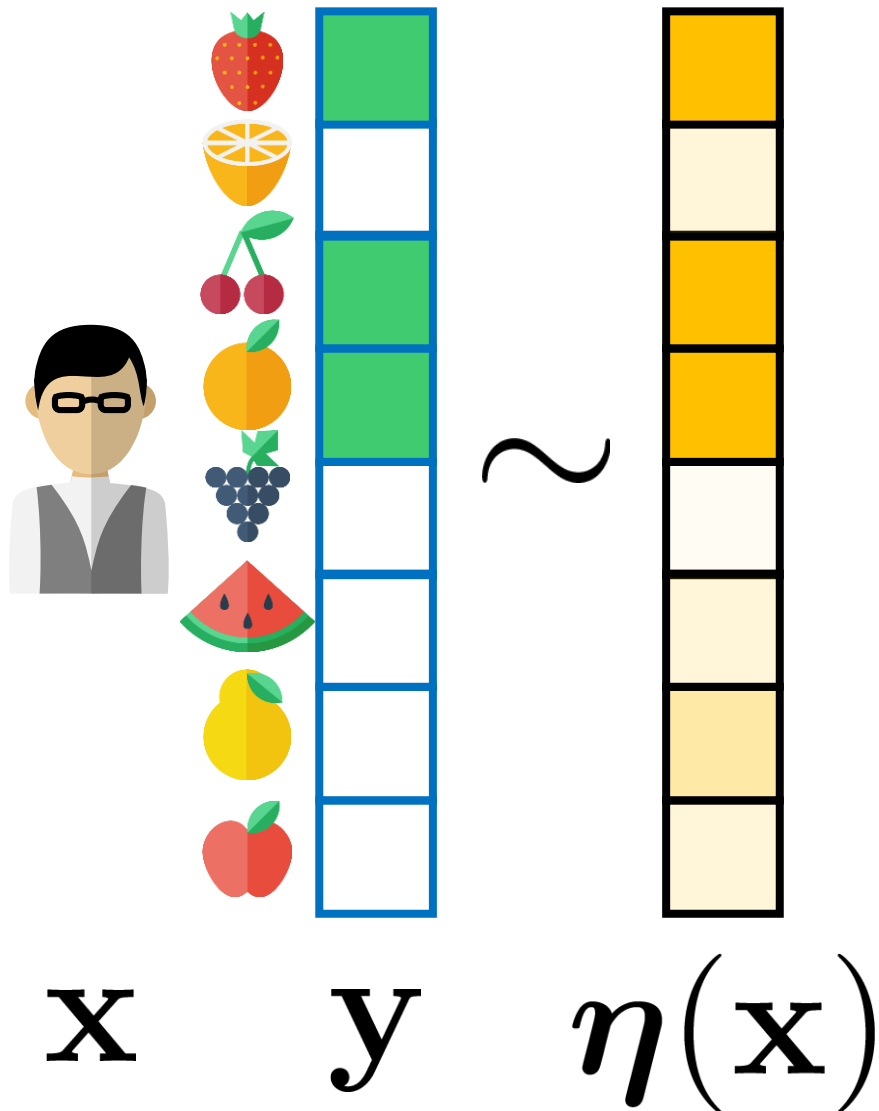
$$\arg \max_{y \in [K]} \langle \mathbf{w}^k, \mathbf{x} \rangle$$

Linear Classifier

Multi-label Learning using PML



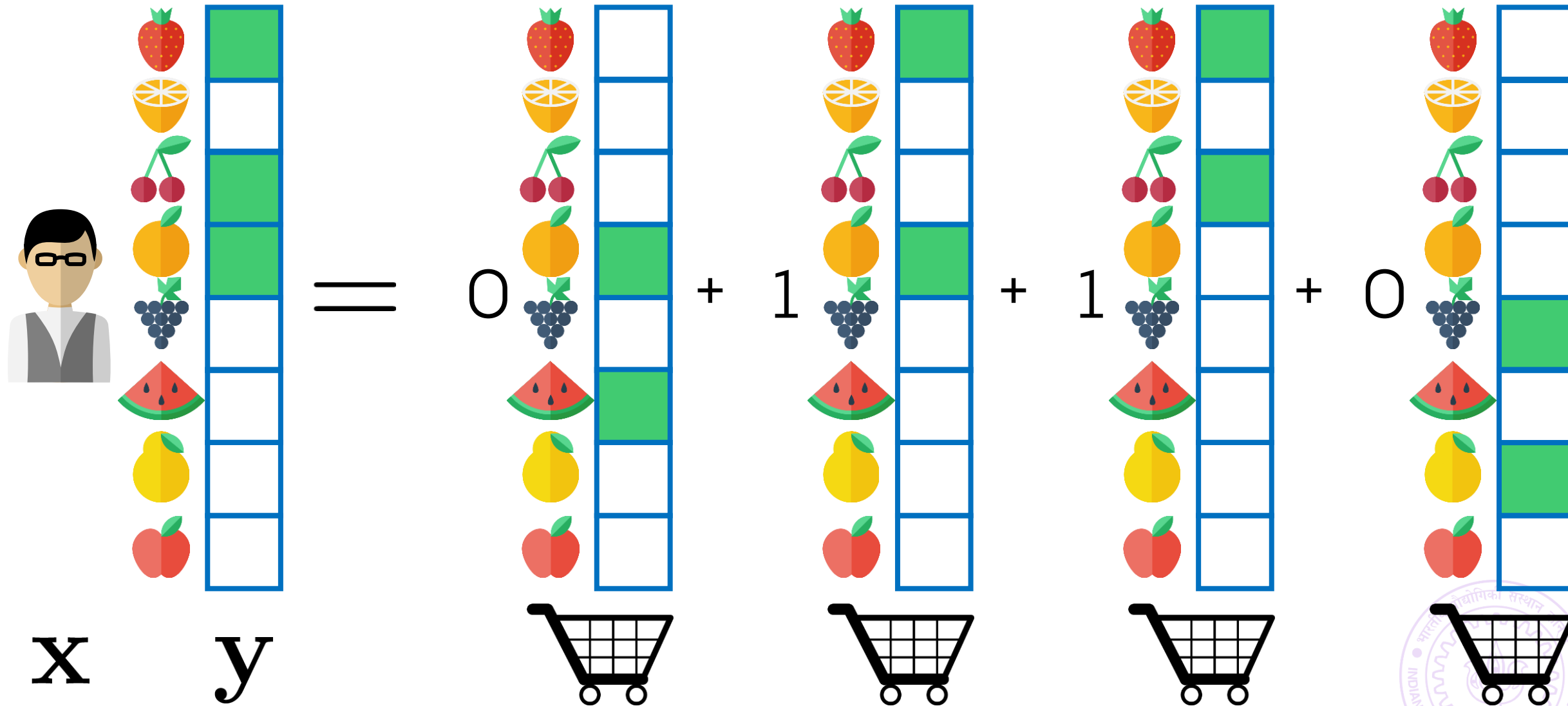
Multi-label Learning using PML



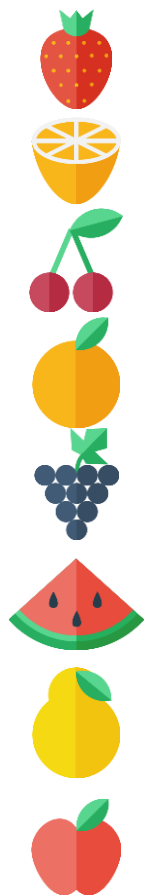
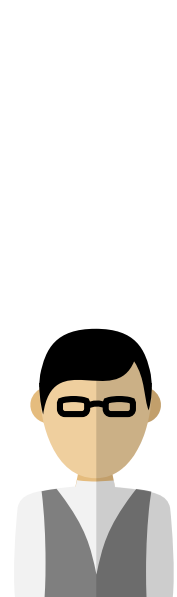
Solve as L independent Binary problems using Logistic regression!

Does not scale!

Multi-label Learning using PML



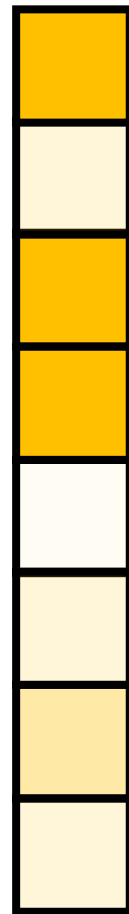
Multi-label Learning using PML



\mathbf{x}

\mathbf{y}

\sim



$\eta(\mathbf{x})$

$=$

\mathbf{u}_1

$+$

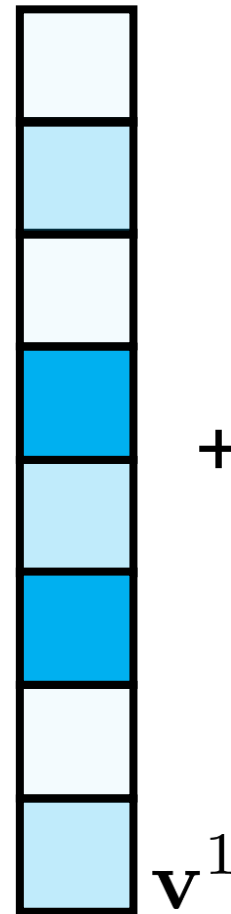
\mathbf{u}_2

$+$

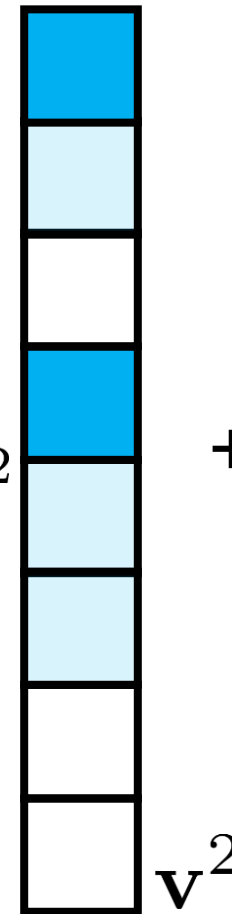
\mathbf{u}_3

$+$

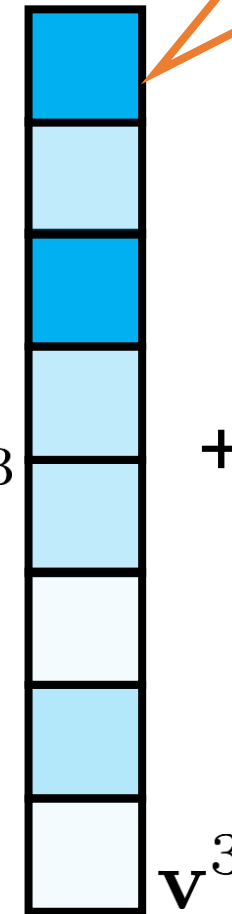
\mathbf{u}_K



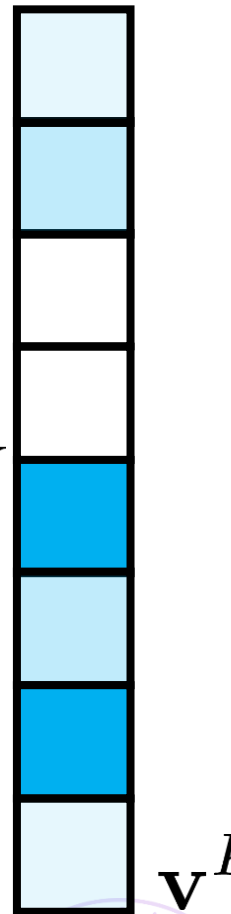
\mathbf{v}^1



\mathbf{v}^2



\mathbf{v}^3



\mathbf{v}^K



Distributions over labels

Multi-label Learning using PML

$$\mathbf{y}^i \sim \text{Bernoulli}(\boldsymbol{\eta}^i)$$

$$\boldsymbol{\eta}^i = \mathbf{V}\mathbf{u}^i, \mathbf{V} = [\mathbf{v}^1, \mathbf{v}^2, \dots, \mathbf{v}^K]$$

$$\mathbf{u}_j^i \sim \mathcal{N}(\langle \mathbf{w}^j, \mathbf{x}^i \rangle, \sigma^2), j = 1, \dots, K$$

Can fix \mathbf{V} or else ...

$$\mathbf{v}^j \sim \text{Dirichlet}(\boldsymbol{\alpha})$$

$$\mathbf{w}^j \sim \mathcal{N}(\mathbf{0}, \rho^2 \cdot I), j = 1, \dots, K$$

Generalization of Beta distribution

$$\mathbb{P}[\mathbf{v}; \boldsymbol{\alpha}] = \frac{1}{B(\boldsymbol{\alpha})} \prod_{i=1}^L \mathbf{v}_i^{\alpha_i - 1}$$

$$\mathbb{P}[p; \alpha, \beta] = \frac{1}{B(\alpha, \beta)} p^{\alpha-1} (1-p)^{\beta-1}$$

Only K models,
not L

Have fun posterioring!

Please give your Feedback

<http://tinyurl.com/ml17-18afb>