Priors and Latent Variables DD2421

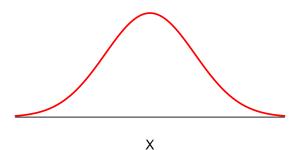
Bob L. T. Sturm

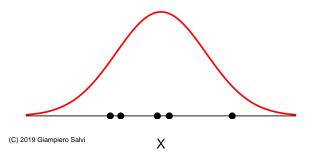
Outline

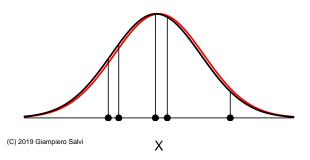
- Incorporating Priors
 - Maximum a Posteriori Estimation
 - Bayesian Non-Parametric Methods
 - Model Selection and Occam's Razor
- Unsupervised Learning
 - Classification vs Clustering
 - Heuristic Example: K-means
 - Expectation Maximization

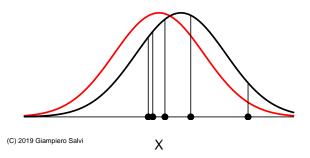
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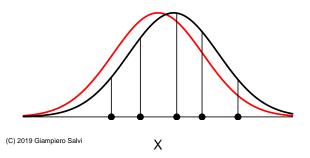
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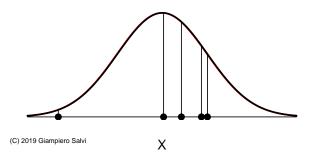


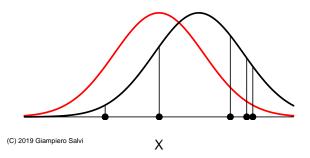


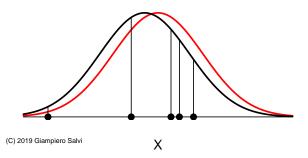


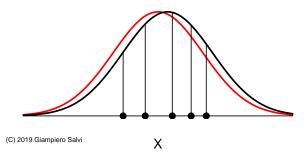


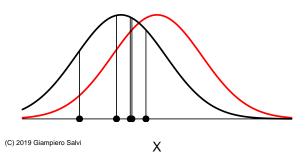


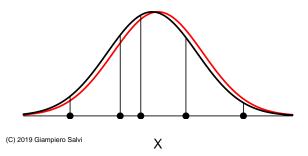


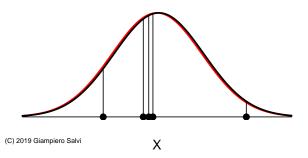


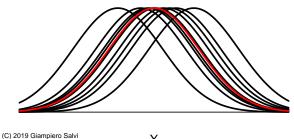












- Recall: ML estimation chooses θ to maximize probability of \mathcal{D} .
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$$= \arg \max_{\theta} \left[\frac{Pr(\theta)}{n} \prod_{n=1}^{N} Pr(x_n|\theta) \right]$$

$$= \arg \max_{\theta} \left[\frac{\log Pr(\theta)}{n} + \sum_{n=1}^{N} \log Pr(x_n|\theta) \right]$$

• $\log Pr(\theta)$ works as a regularizer.

MAP for Linear Regression

Model (deterministic):

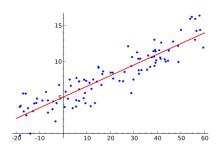
$$y = \mathbf{w}^T \mathbf{x} + \epsilon$$

With:

$$\epsilon \sim \mathcal{N}(0, \sigma_Y^2)$$

Therefore:

$$Y|X \sim \mathcal{N}(\mathbf{w}^T \mathbf{x}, \sigma_Y^2)$$



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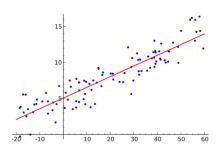
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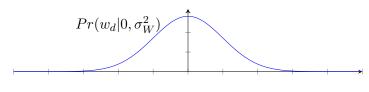
But now we define the a priori probability of \mathbf{w} : $Pr(\mathbf{w})$

We assume in this case $\mathbf{w} \sim \mathcal{N}(\mathbf{0}, \sigma_W^2 \mathbf{I}_D)$

$$Pr(\mathbf{w}|\mathbf{0}, \sigma_W^2) = \frac{1}{(2\pi\sigma_W^2)^{\frac{D}{2}}} \exp\left(-\frac{\mathbf{w}^T\mathbf{w}}{2\sigma_W^2}\right)$$

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$$= \prod_{d=1}^D \frac{1}{\sqrt{2\pi\sigma_W^2}} \exp\left(-\frac{w_d^2}{2\sigma_W^2}\right)$$



$$\mathbf{w}_{\mathsf{MAP}} = \underset{\mathbf{w}}{\operatorname{arg}} \max_{\mathbf{w}} \log Pr(\mathbf{w}|y, x) = \underset{\mathbf{w}}{\operatorname{arg}} \max_{\mathbf{w}} \log \left[Pr(y|x, \mathbf{w}) Pr(\mathbf{w}) \right]$$

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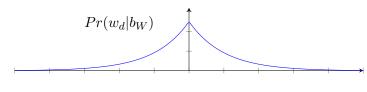
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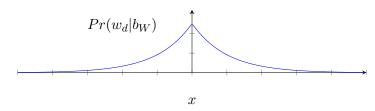
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fit the data (ML)

In this case
$$Pr(\mathbf{w}|\mathbf{b_W}) = \prod_d \frac{1}{2b_W} \exp\left(-\frac{|w_d|}{b_W}\right)$$



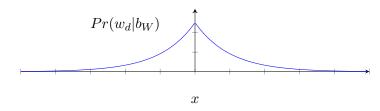
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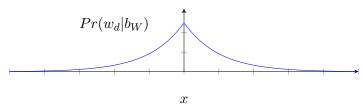
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Impact of different priors

For linear regression $y = \mathbf{w}^T \mathbf{x} + \epsilon$, MAP estimation of \mathbf{w} performs differently considering the prior we assume!

$$\mathbf{w}^*(p) = \arg\min_{\mathbf{w}} \left[\underbrace{\sum_{n=1}^{N} \left(y_n - \mathbf{w}^T \mathbf{x}_n \right)^2}_{\text{fit the data (ML)}} + \underbrace{\lambda \sum_{d=1}^{D} |w_d|^p}_{\text{regularize}} \right]$$

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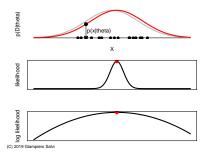
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- $\lambda > 0$ and assuming iid Laplace (p=1): fit the data and make ${\bf w}$ sparse (also know as the Least Absolute Shrinkage and Selection Operator (LASSO))

ML, MAP and Point Estimates

- ullet Both ML and MAP produce point estimates of heta
- Assumption: there is a true value for θ
- ullet advantage: once $\hat{ heta}$ is found, assume everything is known



Limitations (Linear Regression)

- With MAP estimation, the problem shifts to defining the parameters of the prior $Pr(\mathbf{w})$ (equivalently choosing λ in ridge or LASSO regression)
- We still have uncertainty in the posterior $Pr(y|\mathbf{x},\mathbf{w}^*)$ but this is not explicit.
- We don't want $Pr(y|\mathbf{x}, \mathbf{w})$, but instead $Pr(y|\mathbf{x}, \mathcal{D})$.

Bayesian estimation (non-parametric models)

- **①** consider θ as a random variable (same as MAP)
- ② characterize θ with the posterior distribution $Pr(\theta|\mathcal{D})$ given the data
- **3** compute new predicting posterior $Pr(y|\mathbf{x}, \mathcal{D})$ marginalizing over θ (predictive posterior)

$$Pr(y|\mathbf{x}, \mathcal{D}) = \int_{\theta \in \Theta} Pr(y|\mathbf{x}, \theta) Pr(\theta|\mathcal{D}) d\theta$$

Bayesian Linear Regression

Setup:

$$\mathcal{D} = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_N, y_N)\}\$$

Model (same as MAP):

- Y_1, \ldots, Y_n conditionally independent given \mathbf{w}
- $Y|X \sim \mathcal{N}(\mathbf{w}^T \mathbf{x}, \sigma_Y^2)$
- ullet $\mathbf{w} \sim \mathcal{N}(oldsymbol{\mu}_W, oldsymbol{\Sigma}_{oldsymbol{W}}), \quad \mathbf{w} \in \mathbb{R}^D$
- ullet we assume values for σ_Y^2 , $oldsymbol{\mu}_W$, and $oldsymbol{\Sigma_W}$, so $heta \equiv \mathbf{w}$

Goal: Estimate $Pr(y|\mathbf{x}, \mathcal{D})$

Bayesian Linear Regression

$$\begin{split} Pr(y|\mathbf{x},\mathcal{D}) &= \int_{\mathbb{R}^D} Pr(y|\mathbf{x},\mathcal{D},\mathbf{w}) Pr(\mathbf{w}|\mathbf{x},\mathcal{D}) d\mathbf{w} \\ &= \int_{\mathbb{R}^D} Pr(y|\mathbf{x},\mathbf{w}) Pr(\mathbf{w}|\mathcal{D}) d\mathbf{w} \end{split}$$

(assuming $Y|\mathbf{W}=\mathbf{w}$ is independent of \mathcal{D} , and \mathbf{W} is independent of \mathbf{x}). Results obtained with a lot of passages:

- if $Pr(\mathbf{w})$ is Gaussian, then $Pr(\mathbf{w}|\mathcal{D})$ is Gaussian
- since $Pr(y|\mathbf{x}, \mathbf{w})$ is Gaussian, $Pr(y|\mathbf{x}, \mathcal{D})$ is also Gaussian
- Closed-form results in this case.

Find a walk-through of the derivations here

From mathematicalmonk's YouTube channel:

- problem and model definition https://youtu.be/1WvnpjljKXA
- posterior p(w|D), part 1-2
 https://youtu.be/nrd4AnDLR3U
 https://youtu.be/qz2U8coNwV4
- predictive posterior $p(y|\mathbf{x}, \mathcal{D})$, part 1-3 https://youtu.be/xyuSiKXttxw https://youtu.be/vTcsacTqlfQ https://youtu.be/LCISTY9S6SQ

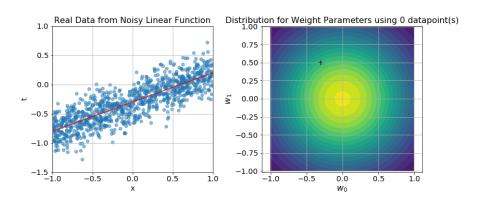
Closed Form Solutions

Define $\Phi^T = [\mathbf{x}_1 | \mathbf{x}_2 | \dots | \mathbf{x}_N]$ and $\mathbf{y} = (y_1, y_2, \dots, y_N)$ from \mathcal{D} . With the assumed set-up, the posterior $\mathbf{w} | \mathcal{D} \sim \mathcal{N}(\boldsymbol{\mu}_{\mathbf{w}|\mathcal{D}}, \boldsymbol{\Sigma}_{\mathbf{w}|\mathcal{D}})$, with:

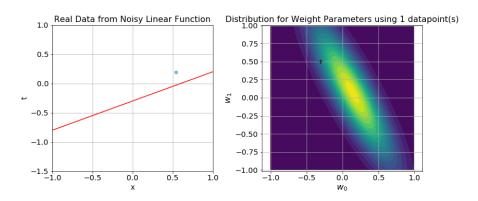
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ight] \end{array}$$

Predictive posterior:

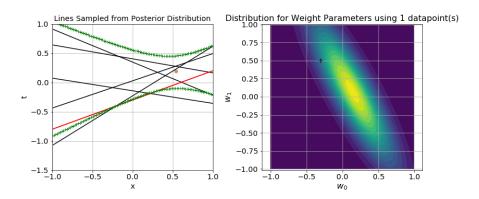
$$Pr(y|\mathbf{x}, \mathcal{D}) = \mathcal{N}(\boldsymbol{\mu}_{\mathbf{w}|\mathcal{D}}^T \mathbf{x}, \sigma_Y^2 + \mathbf{x}^T \boldsymbol{\Sigma}_{\mathbf{w}|\mathcal{D}} \mathbf{x})$$



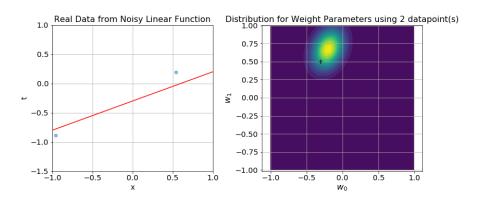
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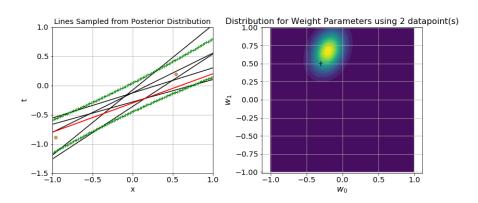
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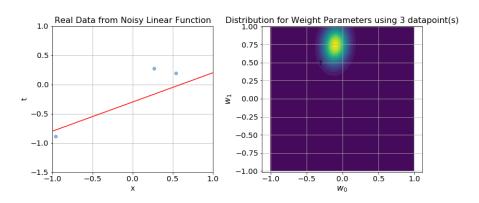
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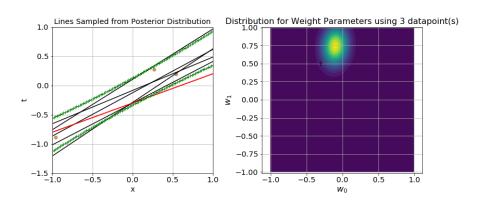
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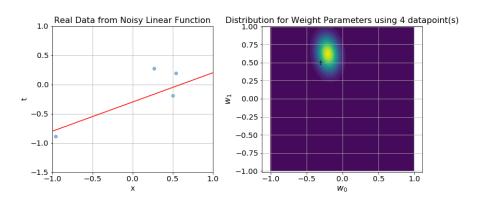
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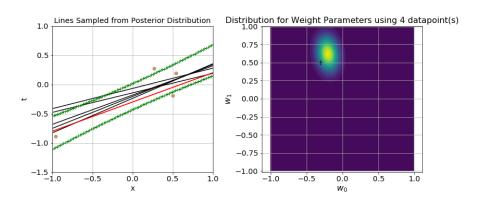
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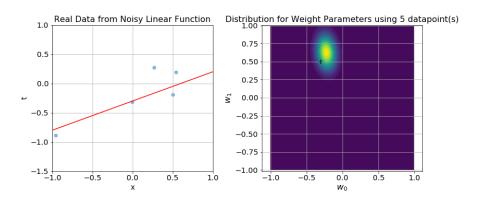
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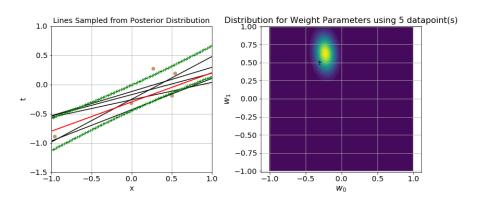
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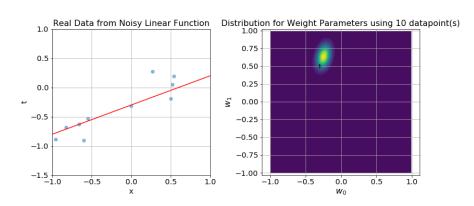
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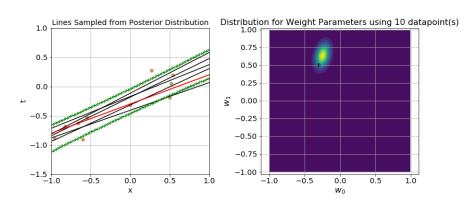
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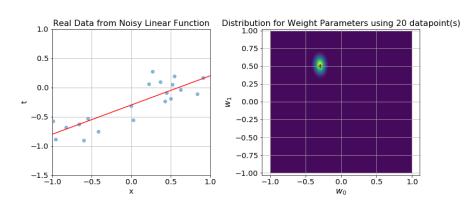
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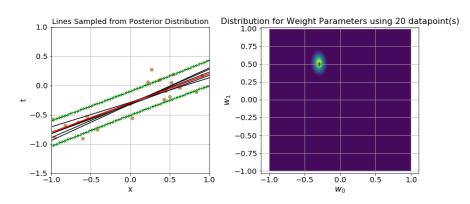
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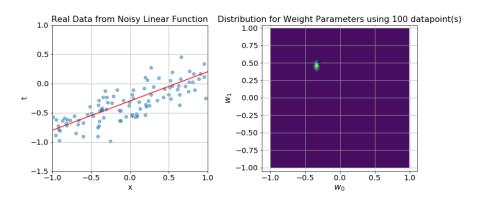
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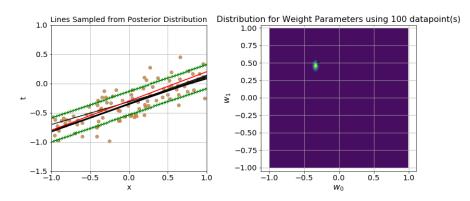
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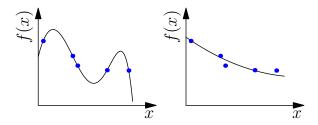
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Consequences

- We are considering the uncertainty over the choice of ${\bf w}$ as well as the original uncertainty σ_Y^2 .
- This provides a means to prevent overfitting



Occam's Razor

Choose the simplest explanation for the observed data

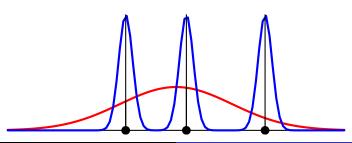
Important factors:

- number of model parameters
- number of data points
- model fit to the data

Overfitting and Maximum Likelihood

$$\theta_{\mathsf{ML}} = \arg\max_{\theta} P(\mathcal{D}|\theta)$$

We can make the likelihood arbitrary large by increasing the number of parameters



Occam's Razor and Bayesian Learning

Remember that:

$$Pr(y|\mathbf{x}, \mathcal{D}) = \int_{\theta \in \Theta} Pr(y|\mathbf{x}, \theta) Pr(\theta|\mathcal{D}) d\theta$$

Occam's Razor and Bayesian Learning

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Intuition:

More complex models fit the data very well (large $Pr(\mathcal{D}|\theta)$ and $Pr(\theta|\mathcal{D})$) but only for small regions of the parameter space Θ .

Limitations of Bayesian Non-parametric Methods

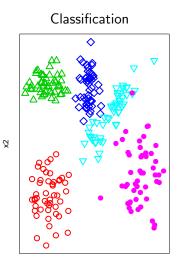
$$Pr(y|\mathbf{x}, \mathcal{D}) = \int_{\mathbb{R}^D} Pr(y|\mathbf{x}, \mathbf{w}) Pr(\mathbf{w}|\mathcal{D}) d\mathbf{w}$$

- closed form solution for $Pr(\mathbf{w}|\mathcal{D})$ is not always possible (conjugate priors)
- can use approximations with high computational cost (sampling methods) or complex solutions (variational methods)
- sometimes we will have a non-informative prior of **W**, but Bayesian methods carry uncertainty estimates.

Outline

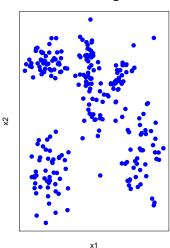
- Incorporating Priors
 - Maximum a Posteriori Estimation
 - Bayesian Non-Parametric Methods
 - Model Selection and Occam's Razor
- Unsupervised Learning
 - Classification vs Clustering
 - Heuristic Example: K-means
 - Expectation Maximization

Clustering vs Classification



x1

Clustering



Heuristic Example: K-means

- describes each class with a centroid
- a point belongs to a class if the corresponding centroid is closest (Euclidean distance)
- iterative procedure
- guaranteed to converge
- not guaranteed to find the optimal solution
- used in *vector quantization* (since the 1950's)

K-means: algorithm

Data: No. of desired clusters K, data set $\mathcal{D} = \{\mathbf{x}_i \in \mathbb{R}^D\}$, distance function $f: \mathbb{R}^D \times \mathbb{R}^D \to \mathbb{R}_+$, threshold ϵ initialization: sample K centroids $\boldsymbol{\mu}_k^{(0)} \in \mathbb{R}^D$ at random; $t \leftarrow 0$; repeat

assign each point x_i to closest centroid:

$$C_k := \left\{ \mathbf{x} \in \mathcal{D} : k = \arg\min_{k'} f(\mathbf{x}, \boldsymbol{\mu}_{k'}^{(t)}) \right\}$$

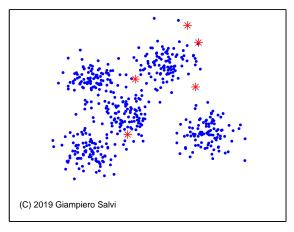
update centroids as mean of each cluster of points:

$$\boldsymbol{\mu}_k^{(t+1)} = rac{1}{|\mathcal{C}_k|} \sum \mathcal{C}_k$$

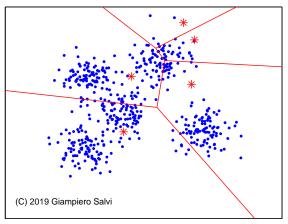
iterate $t \leftarrow t+1$ until $\max_k f(\boldsymbol{\mu}_k^{(t-1)}, \boldsymbol{\mu}_k^{(t)}) < \epsilon$; return K clusters of data points.

K-means: example

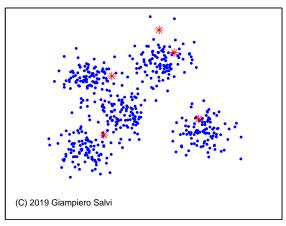
initialization



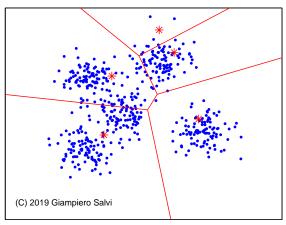
iteration 1, update clusters



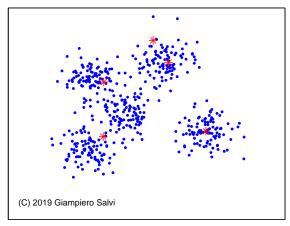
iteration 2, update centroids



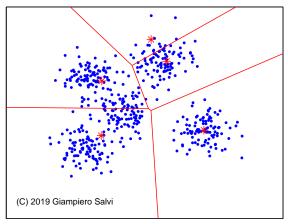
iteration 2, update clusters



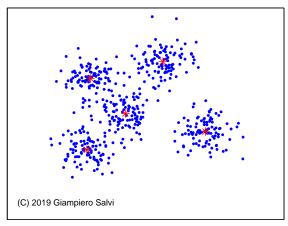
iteration 3, update centroids



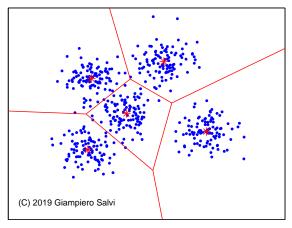
iteration 3, update clusters



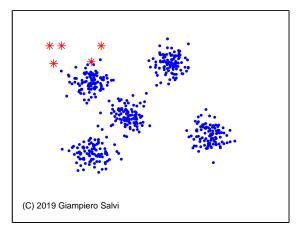
iteration 20, update centroids



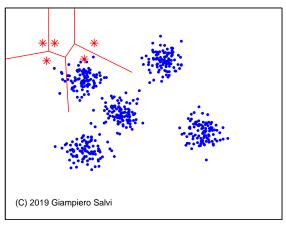
iteration 20, update clusters



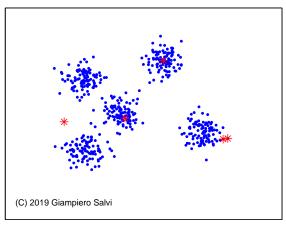
initialization



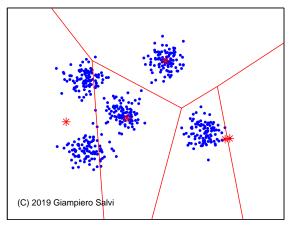
iteration 1, update clusters



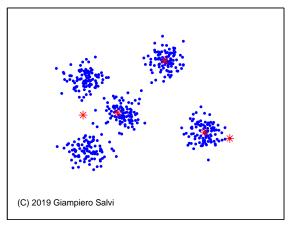
iteration 2, update centroids



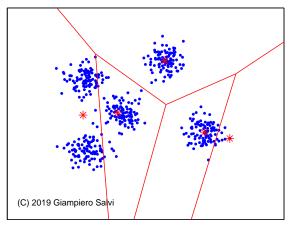
iteration 2, update clusters



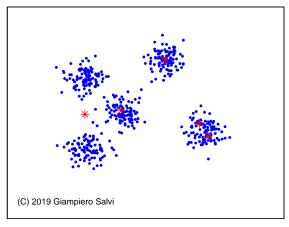
iteration 3, update centroids



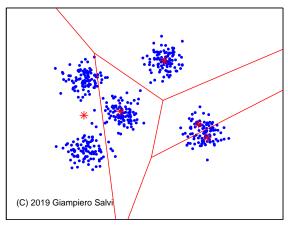
iteration 3, update clusters



iteration 20, update centroids



iteration 20, update clusters

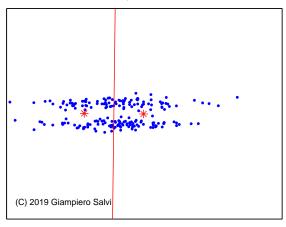


K-means: limits of Euclidean distance

- ullet the Euclidean distance is isotropic (same in all directions in \mathbb{R}^p)
- this favors spherical clusters
- the size of the clusters is controlled by the distances between them

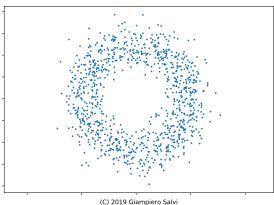
K-means: non-spherical classes

two non-spherical classes



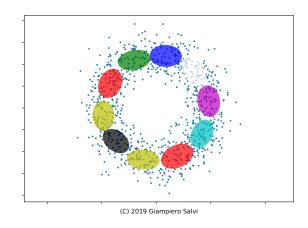
Example: doughnut data

$$\mathcal{D} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$$



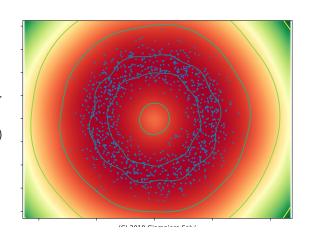
Example: doughnut data

$$\mathcal{D} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$$
$$Pr(\mathbf{x}|\theta_k), \forall k \in [1, K]$$



Example: doughnut data

$$\mathcal{D} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$$
$$Pr(\mathbf{x}|\theta) = \sum_{k=1}^K \pi_k Pr(x|\theta_k)$$



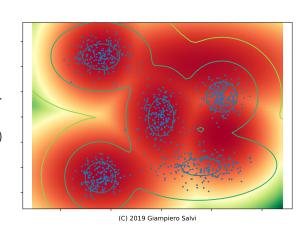
Clustering Example

$$\mathcal{D} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$$



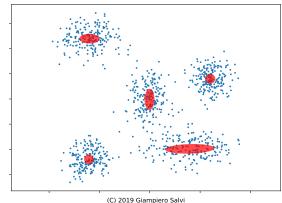
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Clustering Example

$$\mathcal{D} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$$
$$Pr(\mathbf{x}|\theta_k), \forall k \in [1, K]$$



Fitting complex distributions

We can try to fit a mixture of K distributions:

$$Pr(\mathbf{x}|\theta) = \sum_{k=1}^{K} \pi_k Pr(\mathbf{x}|\theta_k)$$

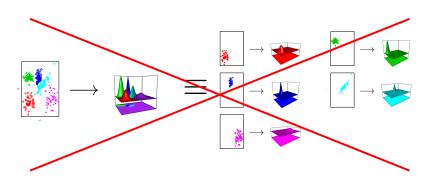
with
$$\theta = \{\pi_1, \dots, \pi_k, \theta_1, \dots, \theta_K\}$$

Problem:

We do not know which point has been generated by which component of the mixture

We cannot optimize $Pr(\mathbf{x}|\theta)$ directly

No Class Independence Assumption



Solution: Expectation Maximization

Expectation Maximization

Fitting model parameters with missing (latent) variables

$$Pr(\mathbf{x}|\theta) = \sum_{k=1}^{K} \pi_k Pr(\mathbf{x}|\theta_k),$$

with
$$\theta = \{\pi_1, \dots, \pi_k, \theta_1, \dots, \theta_K\}$$

- very general idea (applies to many different probabilistic models)
- augment data with latent variables: $h_i \in \{1, \dots, K\}$ is the assignment of data point x_i to a component of the mixture
- ullet optimize likelihood of the complete data over N data points

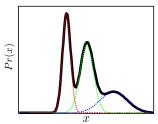
$$Pr(\mathbf{x}_1,\ldots,\mathbf{x}_N,h_1,\ldots,h_N|\theta)$$

Example: Mixture of Gaussians

This distribution is a weighted sum of K Gaussian distributions

$$Pr(x) = \sum_{k=1}^{K} \pi_k \mathcal{N}(x|\mu_k, \sigma_k^2)$$

where
$$\pi_1 + \cdots + \pi_K = 1$$
, $\pi_k > 0$ $(k = 1, \dots, K)$.



This model can describe **complex multi-modal** probability distributions by combining simpler distributions.

Mixture of Gaussians as a marginalization

We can interpret the Mixture of Gaussians model with the introduction of a discrete hidden/latent variable h and Pr(x,h):

$$Pr(x) = \sum_{k=1}^{K} Pr(x, h = k) = \sum_{k=1}^{K} Pr(x \mid h = k) Pr(h = k)$$

$$= \sum_{k=1}^{K} \pi_k \mathcal{N}(x \mid \mu_k, \sigma_k^2)$$

$$\leftarrow \text{mixture density}$$

Figures taken from Computer Vision: models, learning and inference by Simon Prince,

EM for two Gaussians

For each sample x_i introduce a hidden variable h_i

$$h_i = \begin{cases} 1 & \text{if sample } x_i \text{ was drawn from } \mathcal{N}(x|\mu_1, \sigma_1^2) \\ 2 & \text{if sample } x_i \text{ was drawn from } \mathcal{N}(x|\mu_2, \sigma_2^2) \end{cases}$$

and come up with initial values

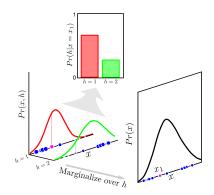
$$\Theta^{(0)} = (\pi_1^{(0)}, \mu_1^{(0)}, \sigma_1^{(0)}, \mu_2^{(0)}, \sigma_2^{(0)})$$

for each of the parameters.

EM is an *iterative algorithm* which updates $\Theta^{(t)}$ using the following two steps...

EM for two Gaussians: E-step

The responsibility of k-th Gaussian for each sample x (indicated by the size of the projected data point)



Look at each sample \boldsymbol{x} along hidden variable \boldsymbol{h} in the E-step

Figure from Computer Vision: models, learning and inference by Simon Prince.

EM for two Gaussians: E-step (cont.)

E-step: Compute the posterior probability (*responsibility*) that x_i was generated by component k given the current estimate of the parameters $\Theta^{(t)}$.

for each data point $i = 1, \dots, N$

for each mixture component k = 1, 2

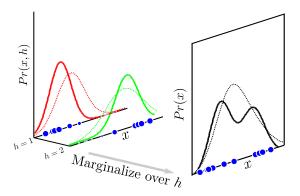
$$\gamma_{ik}^{(t)} := Pr(h_i = k \mid x_i, \Theta^{(t)}) = \frac{Pr(h_i = k, \Theta^{(t)}) Pr(x_i \mid h_i = k, \Theta^{(t)})}{Pr(x_i \mid \Theta^{(t)})}$$

$$= \frac{\pi_k^{(t)} \mathcal{N}(x_i \mid \mu_k^{(t)}, \sigma_k^{(t)})}{\pi_1^{(t)} \mathcal{N}(x_i \mid \mu_1^{(t)}, \sigma_1^{(t)}) + \pi_2^{(t)} \mathcal{N}(x_i \mid \mu_2^{(t)}, \sigma_2^{(t)})}$$

Note: Responsibilities $\gamma_{i1}^{(t)} + \gamma_{i2}^{(t)} = 1$ and mixture weights $\pi_1 + \pi_2 = 1$

EM for two Gaussians: M-step

Fitting the Gaussian model for each of k-th constinuent. Sample x_i contributes according to the *responsibility* γ_{ik} .



(dashed and solid lines for fit before and after update)

Look along samples x for each h in the M-step

EM for two Gaussians: M-step (cont.)

M-step: Compute the maximum likelihood estimates of $\Theta^{(t)}$ given the data membership distributions (the $\gamma_{i1}^{(t)}$, $\gamma_{i2}^{(t)}$):

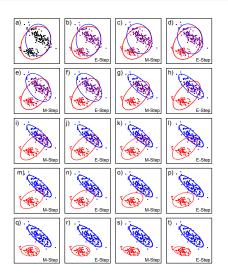
for
$$k = 1, 2$$

$$\mu_k^{(t+1)} = \frac{\sum_{i=1}^N \gamma_{ik}^{(t)} x_i}{\sum_{i=1}^N \gamma_{ik}^{(t)}}$$

$$\sigma_k^{(t+1)} = \sqrt{\frac{\sum_{i=1}^N \gamma_{ik}^{(t)} (x_i - \mu_k^{(t+1)})^2}{\sum_{i=1}^N \gamma_{ik}^{(t)}}}$$

$$\pi_k^{(t+1)} = \frac{\sum_{i=1}^{N} \gamma_{ik}^{(t)}}{N}$$

EM in practice



EM properties

Similar to K-means

- guaranteed to find a local maximum of the complete data likelihood
- somewhat sensitive to initial conditions

Better than K-means

- Gaussian distributions can model clusters with different shapes
- all data points are smoothly used to update all parameters
- ullet Can include a prior $Pr(\Theta)$ to introduce regularization

Summary

- Incorporating Priors
 - Maximum a Posteriori Estimation
 - Bayesian Non-Parametric Methods
 - Model Selection and Occam's Razor
- 2 Unsupervised Learning
 - Classification vs Clustering
 - Heuristic Example: K-means
 - Expectation Maximization