Chapter 6 : Functional Data Fusion Application to Supervised Learning

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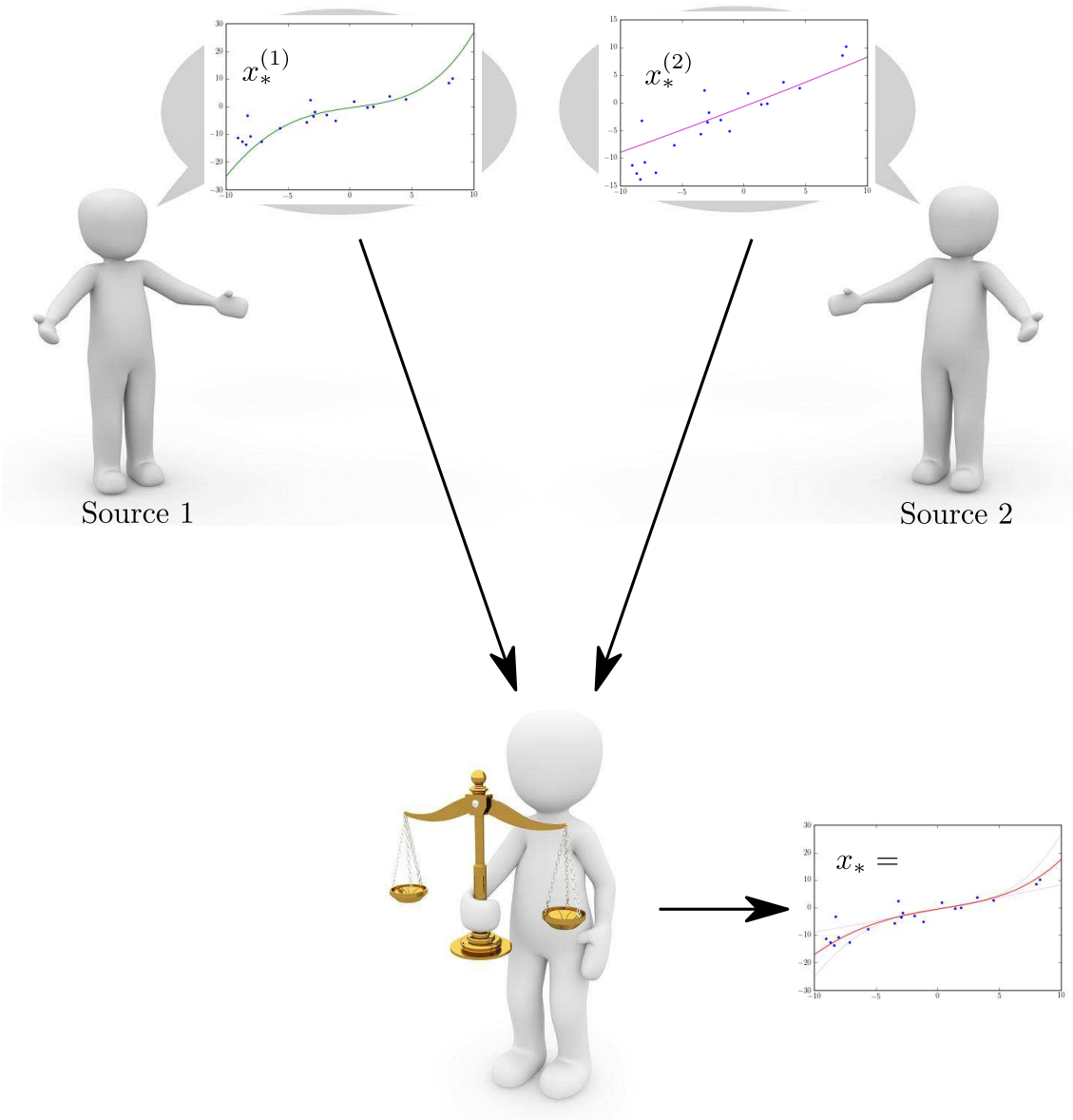
Chapter organization

- In this chapter, each datum delivered by a source is a **function**.

- We focus on regression or classification functions in a supervised learning paradigm.

Probabilistic data fusion setting :



Functional data fusion :

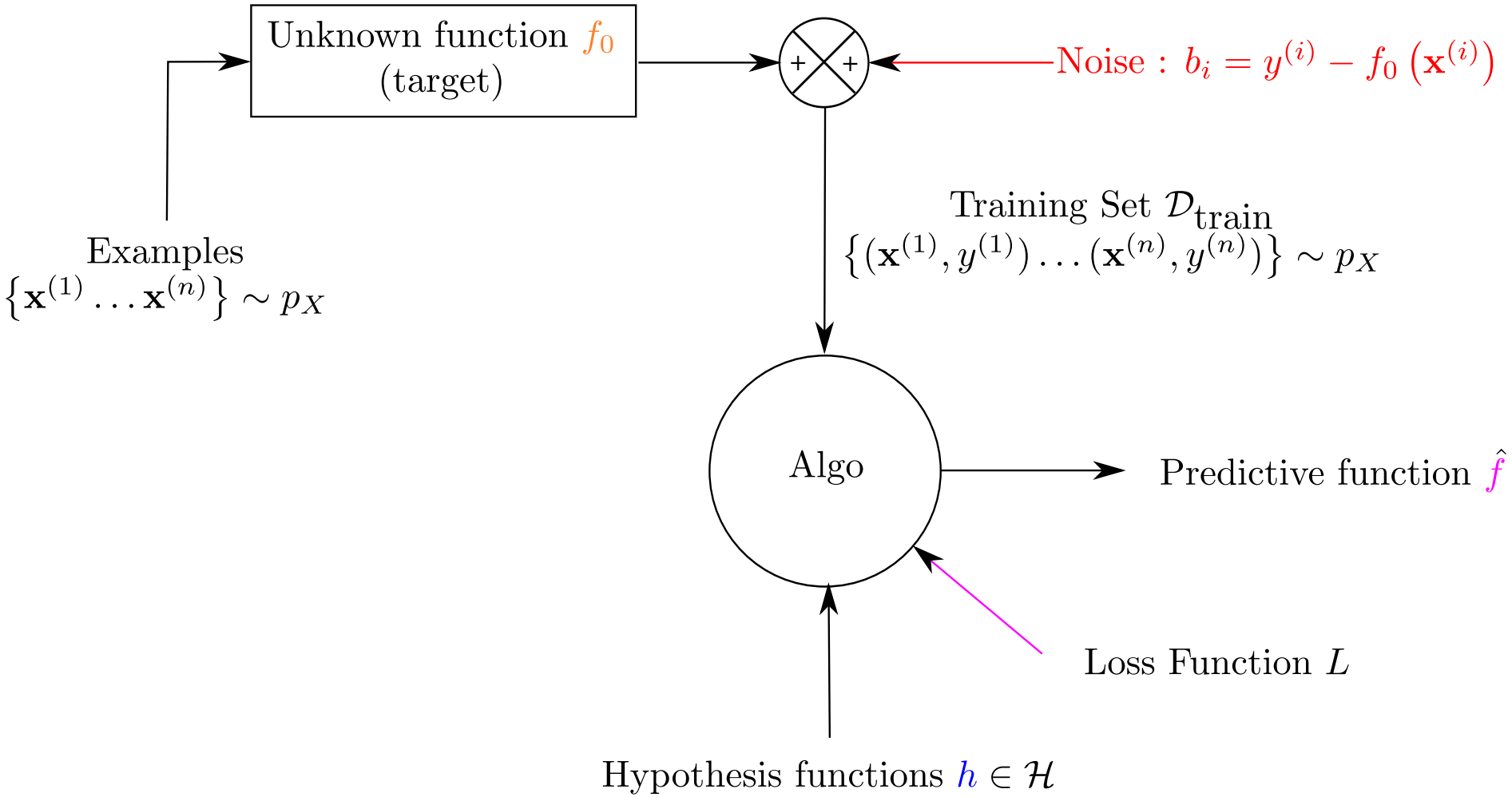
- Let $\mathcal{L}_2$ denote the space of square integrable functions.

- Let us give a formal definition of functional data fusion problems :

Definition

Functional data fusion is a subclass of data fusion where advocacies live in $\mathbb{X} = \mathcal{L}_2$.

Supervised Learning : the learning diagram



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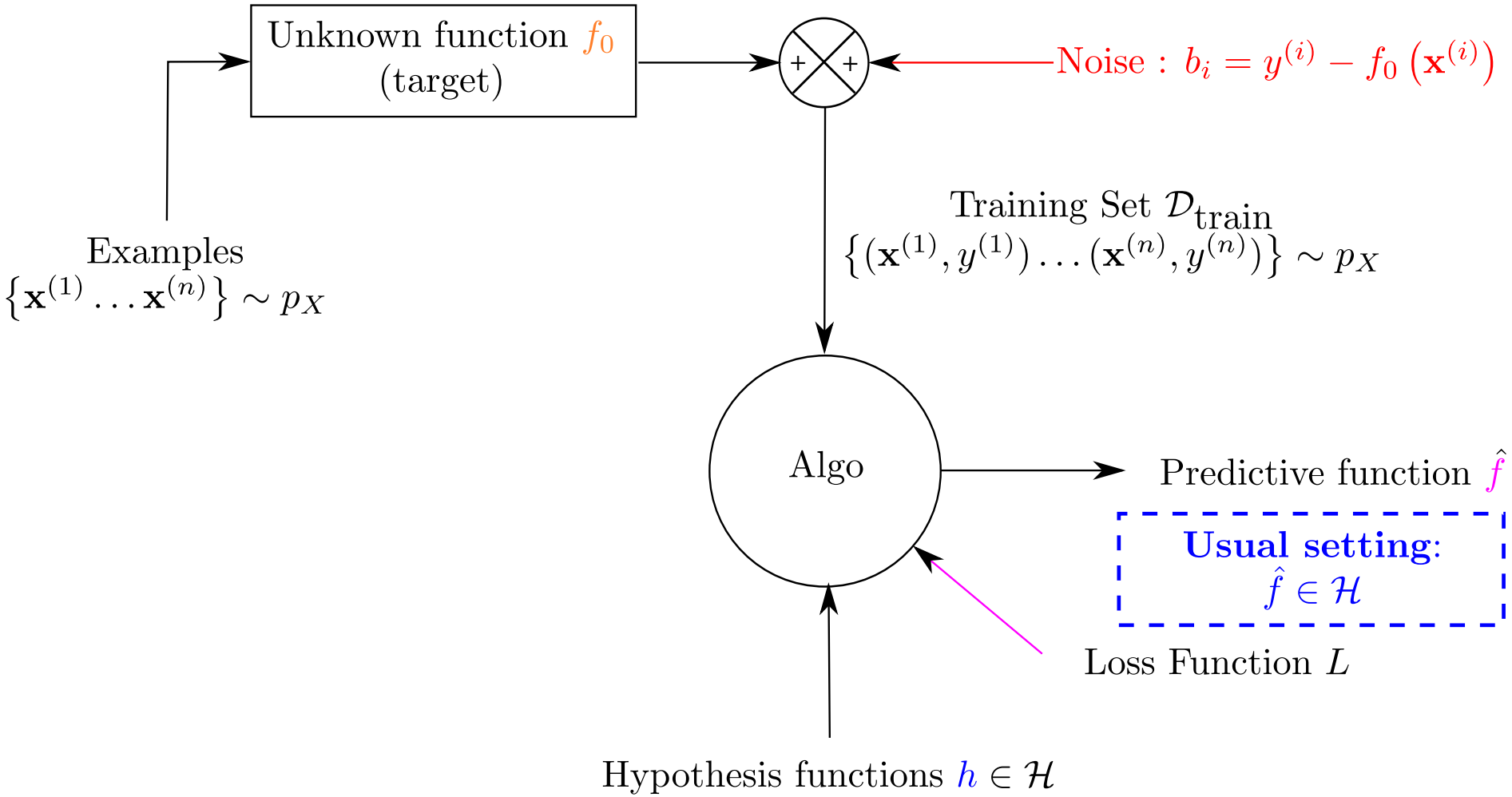
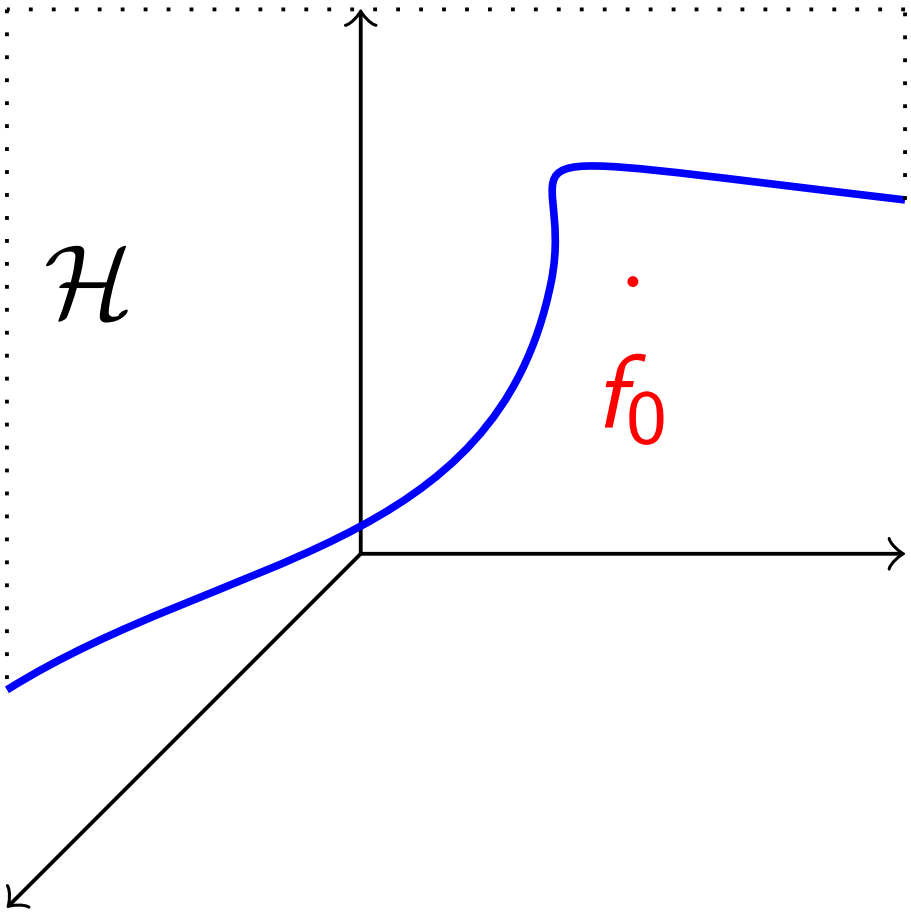
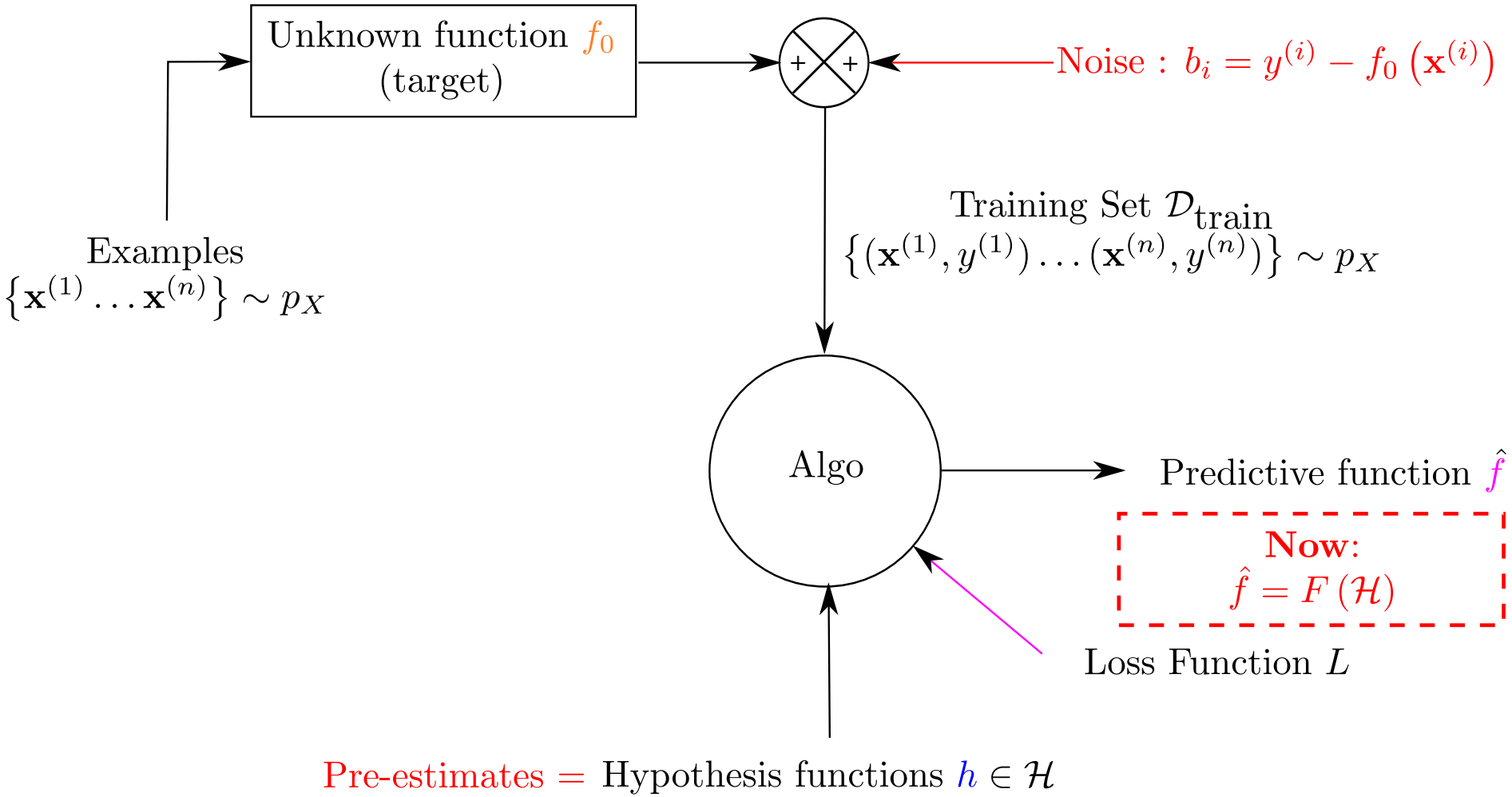


Supervised Learning :

- Notion of hypothesis set $\mathcal{H}$ of prediction functions

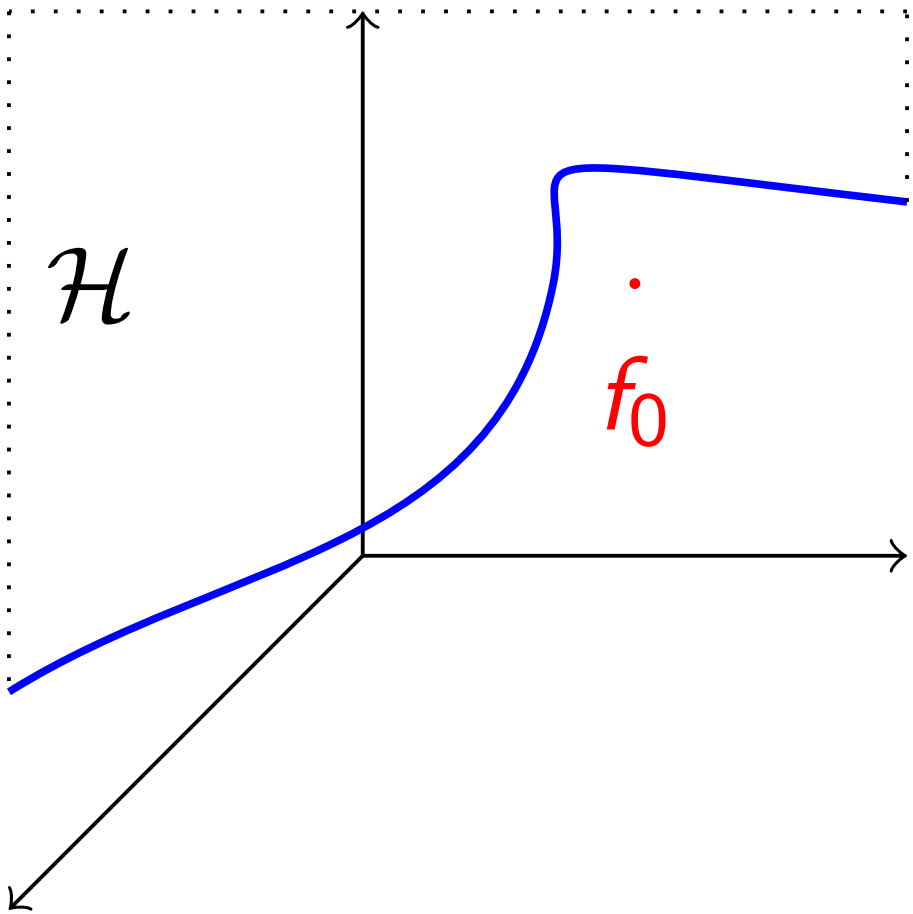


Supervised Learning : the learning diagram



Supervised Learning :

- No free lunch : higher learning capacity $\rightarrow$ more parameters to learn !

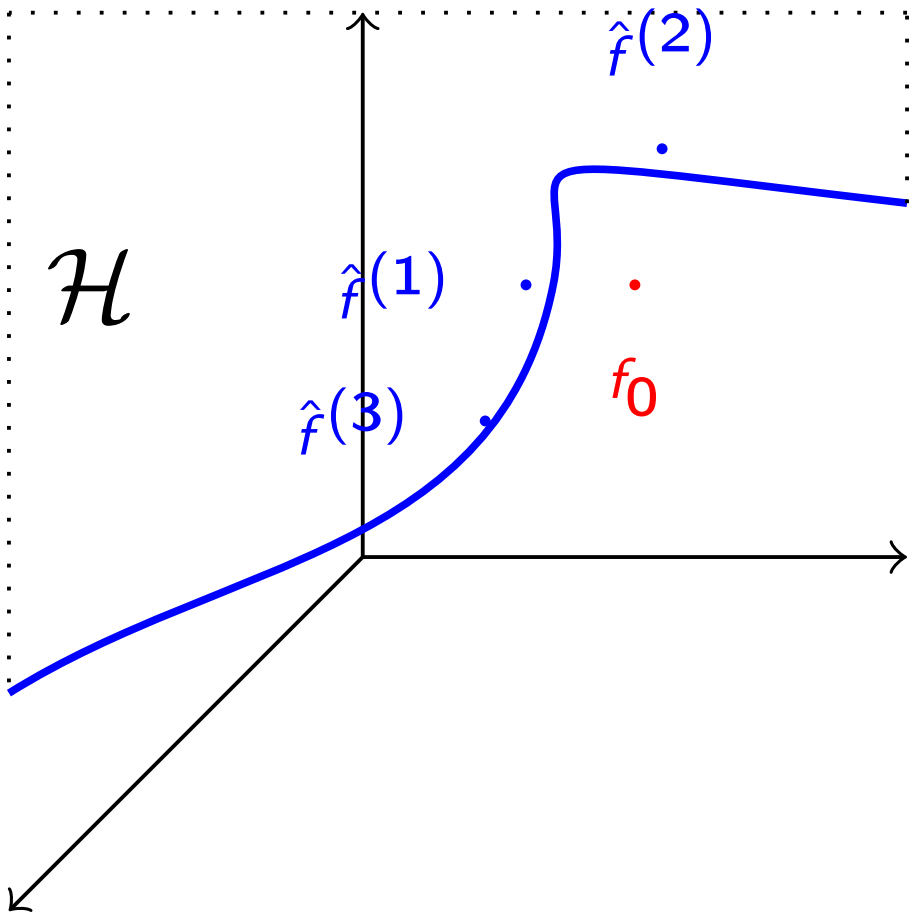


New notations :

Before	Now
x (solution)	f_0 (solution)
x_* (aggregate)	$\hat{f}$ (aggregated estimate)
$x_*^{(i)}$ (advocacy)	$\hat{f}_i$ (pre-estimates)

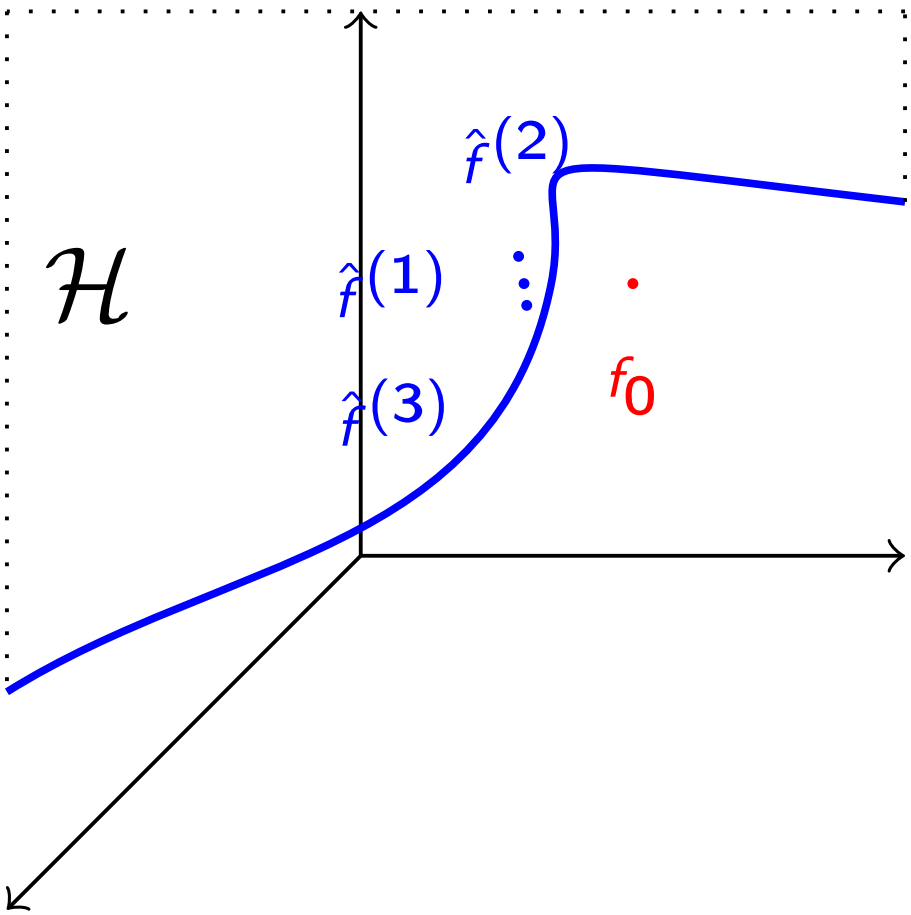
Combining predictors :

- We want diversity in the $\hat{f}^{(i)}$:



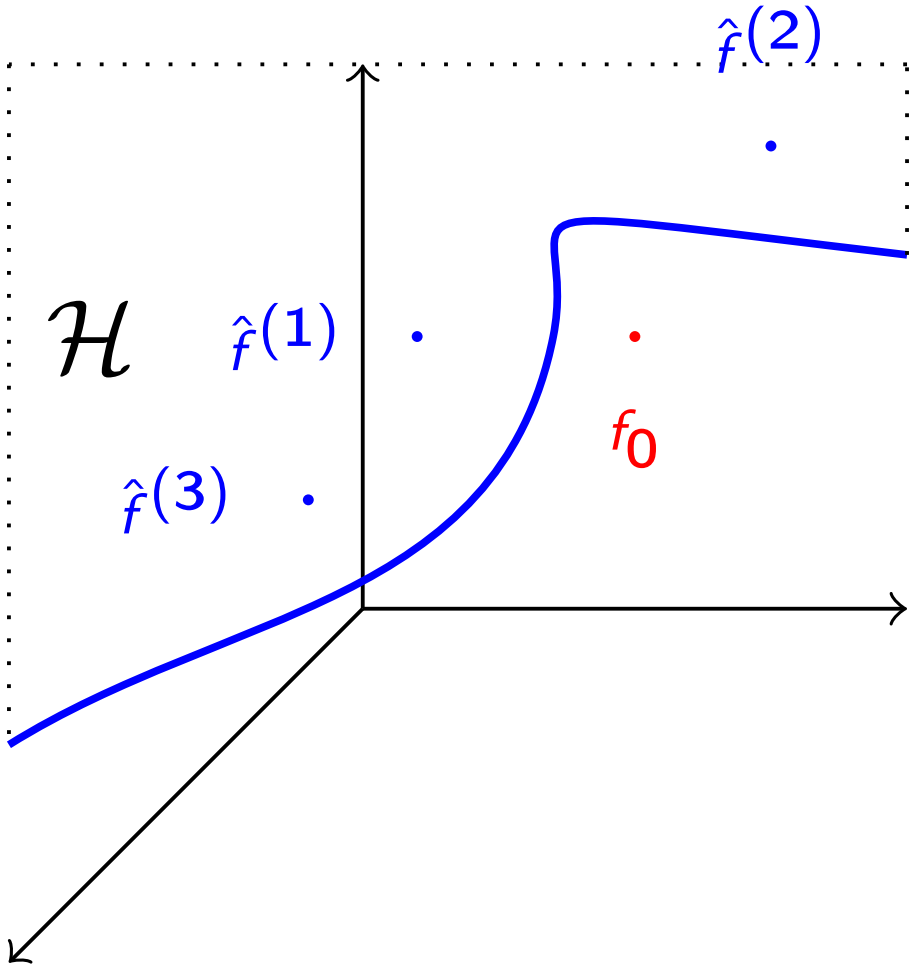
Combining predictors :

- We don't want consanguinity in the $\hat{f}^{(i)}$:



Combining predictors :

- We also don't want bad individual accuracy for the $\hat{f}^{(i)}$:



Supervised Learning : important notions

- Train Error (empirical risk) :

$$E_{\text{train}} = \sum_{i=1}^{n} L\left(\hat{f}\left(\mathbf{x}^{(i)}\right), y^{(i)}\right) = \sum_{\left(\mathbf{x}^{(i)}, y^{(i)}\right) \in \mathcal{D}_{\text{train}}} L\left(\hat{f}\left(\mathbf{x}^{(i)}\right), y^{(i)}\right).$$

- Test Error :

$$E_{\text{test}} = \sum_{\left(\mathbf{x}^{(i)}, y^{(i)}\right) \in \mathcal{D}_{\text{test}}} L\left(\hat{f}\left(\mathbf{x}^{(i)}\right), y^{(i)}\right).$$

- Out of sample Error :

$$E_{\text{out}} = \mathbb{E}_{(X,Y)}\left[L\left(\hat{f}\left(.\right), .\right)\right].$$

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Supervised Learning : important notions

- Err_{train} is a biased estimator of E_{out}.
- Err_{test} is a unbiased estimator of E_{out}.
- If $\hat{f}$ is learnt from $\mathcal{D}_{\text{train}}$, then the genuine model error is :

$$E_{\text{mod}} = \mathbb{E}_{\mathcal{D}}\left[\mathbb{E}_{(X,Y)}\left[L\left(\hat{f}\left(.\right),.\right)\right]\right].$$

- It features the ability for the algorithm to generalize correctly in this situation while the previous definition features only the ability of the output predictor $\hat{f}$ to generalize.

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Chapter organization

Mixture models : definition

- A mixture model is a convex combination of posterior (predictive) distributions $p_{Y|X;\theta_i}(y|\mathbf{x})$:

$$p_{Y|X;\Theta}(y|\mathbf{x}) = \sum_{i=1}^{N_s} \pi_i p_{Y|X;\theta_i}(y|\mathbf{x})$$

- The combined distribution depends on the sources parameters θ_i and the combination parameters π_i :

$$\Theta = \{\theta_1, \ldots, \theta_{N_s}, \pi_1, \ldots, \pi_{N_s}\}.$$

- We have $\sum_{i=1}^{N_s} \pi_i = 1$ and $\pi_i \geq 0, \forall i$.

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- Consequently, the aggregated estimate is obtained by a weighted vote.
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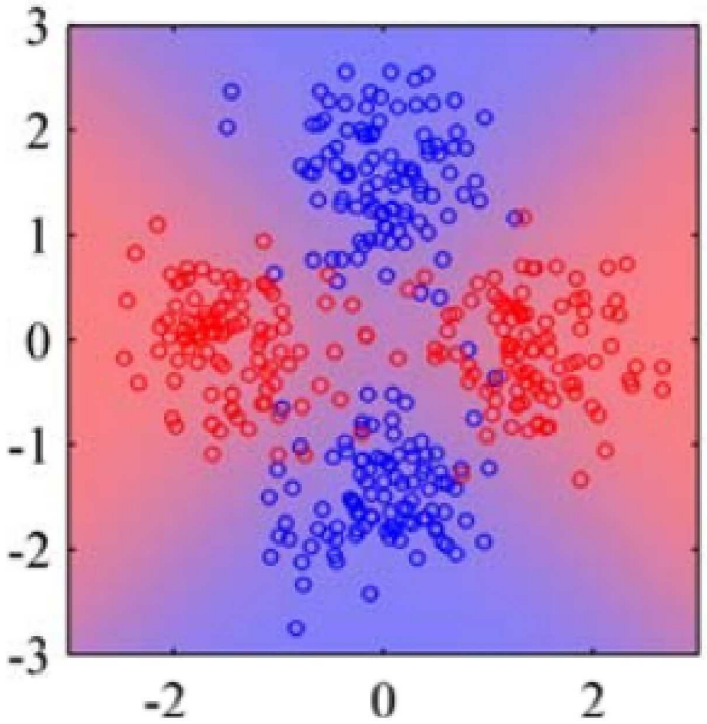
Mixture models : Example - Mixture of LogRegs

- Impossible to fit a linear model to this dataset :



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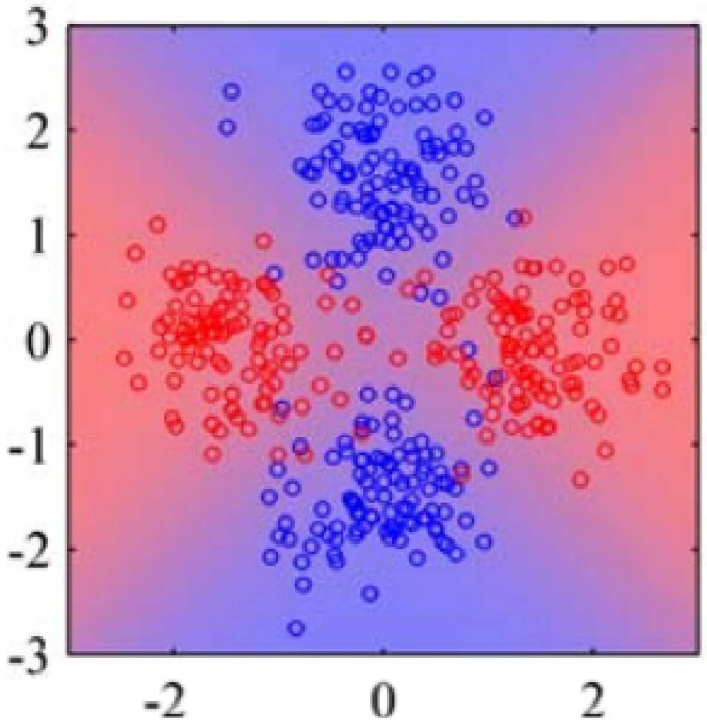

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- Outputs y are binary variables $\{0; 1\}$ and inputs $\mathbf{x}$ are vectors in $\mathbb{R}^d$.

- The posterior is :

$$p_{Y|X;\Theta}(y|\mathbf{x}) = \pi_1 (1-\hat{y}_1)^{1-y} \hat{y}_1^y + \pi_2 (1-\hat{y}_2)^{1-y} \hat{y}_2^y,$$
$$= \begin{cases} \pi_1 \hat{y}_1 + \pi_2 \hat{y}_2 & \text{if } y = 1 \\ \pi_1 (1-\hat{y}_1) + \pi_2 (1-\hat{y}_2) & \text{if } y = 0 \end{cases},$$

with $\hat{y}_1 = \text{sgm}\left(\boldsymbol{\theta}_1^T \cdot \mathbf{x}_+\right)$ and $\hat{y}_2 = \text{sgm}\left(\boldsymbol{\theta}_2^T \cdot \mathbf{x}_+\right)$ the logitic outputs and

$$\mathbf{x}_+^{(i)} = \begin{bmatrix} x_1^{(i)} \\ \vdots \\ x_d^{(i)} \\ 1 \end{bmatrix}$$

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- The likelihood is

$$
\begin{aligned}
\mathcal{L}(\boldsymbol{\Theta}) &= p(\text{data}|\boldsymbol{\Theta}), \\
&= \prod_{i=1}^{n} p(\text{datum number } i|\boldsymbol{\Theta}), \\
&= \prod_{i=1}^{n} p_{Y|X=\mathbf{x}^{(i)};\boldsymbol{\Theta}}\left(y^{(i)}\right), \\
&= \prod_{i=1}^{n} \pi_1 \left(1-\hat{y}_1^{(i)}\right)^{1-y^{(i)}} \left(\hat{y}_1^{(i)}\right)^{y^{(i)}} + \pi_2 \left(1-\hat{y}_2^{(i)}\right)^{1-y^{(i)}} \left(\hat{y}_2^{(i)}\right)^{y^{(i)}}.
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- Let us introduce latent variables $z^{(i)} \in \{1; 2\}$ standing for the fact that example $\mathbf{x}^{(i)}$ was generated by mixture component number.
- $z^{(i)} \sim \text{Ber}(\pi_2)$: $P\left(z^{(i)} = 1\right) = \pi_1$ and $P\left(z^{(i)} = 2\right) = \pi_2 = 1 - \pi_1$.
- The complete data [1] likelihood is then :

$$\begin{aligned} \mathcal{L}_{\text{comp}}(\Theta) &= \prod_{i=1}^{n} p\left(y^{(i)}, z^{(i)} | \mathbf{x}^{(i)}, \Theta\right), \\ &= \prod_{i=1}^{n} \prod_{k=1}^{2} \left(\pi_k \left(1 - \hat{y}_k^{(i)}\right)^{1-y^{(i)}} \left(\hat{y}_k^{(i)}\right)^{y^{(i)}}\right)^{\mathbb{I}_k\left(z^{(i)}\right)}. \end{aligned}$$

- A fake multiplication appears because now each point is concerned with only one component of the mixture !

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- E step : one can show that

$$\mathbb{E}_{\substack{z^{(1)},..,z^{(n)} \\ |\mathcal{D};\Theta}}\left[\log \mathcal{L}_{\text{comp}}\left(\Theta\right)\right] = \sum_{i=1}^{n}\sum_{k=1}^{2}\gamma_k^{(i)}\left[\log\left(\pi_k\right) + \left(1-y^{(i)}\right)\log\left(1-\hat{y}_k^{(i)}\right) + y^{(i)}\log\left(\hat{y}_k^{(i)}\right)\right],$$

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- M step : parameters θ_j need to be estimated using a gradient ascent (Newton's method) while mixing weights are given by :

$$\pi_k = \frac{1}{n}\sum_{i=1}^{n}\gamma_k^{(i)}.$$

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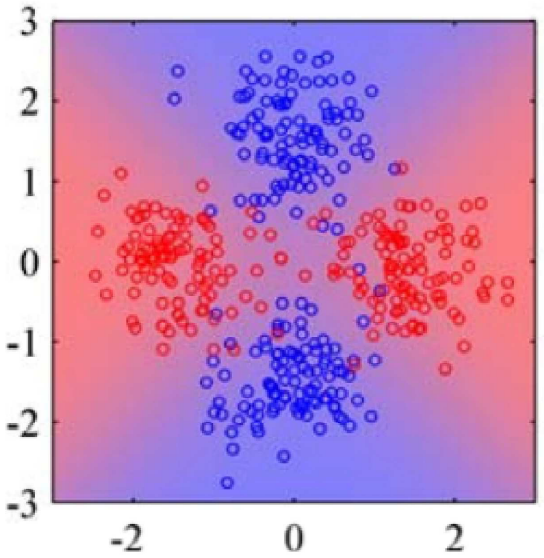
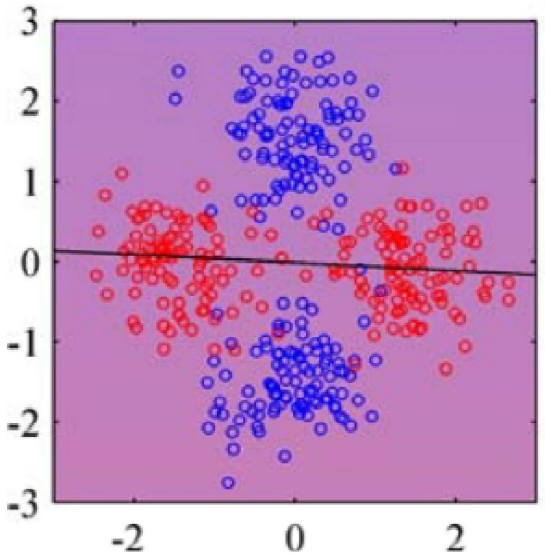
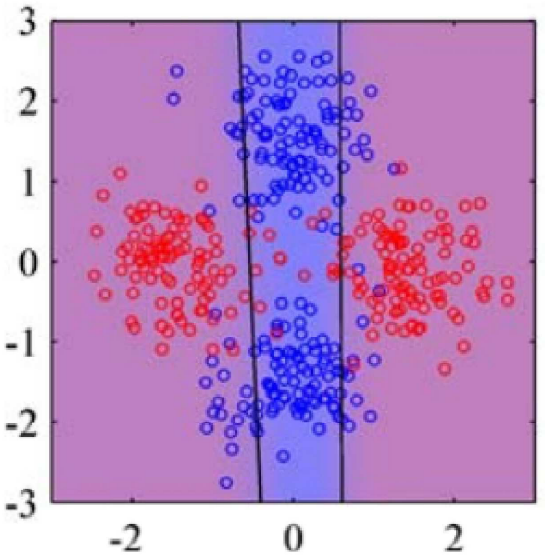
- The fit result is







- See [Bishop 14.5.2] for more details.

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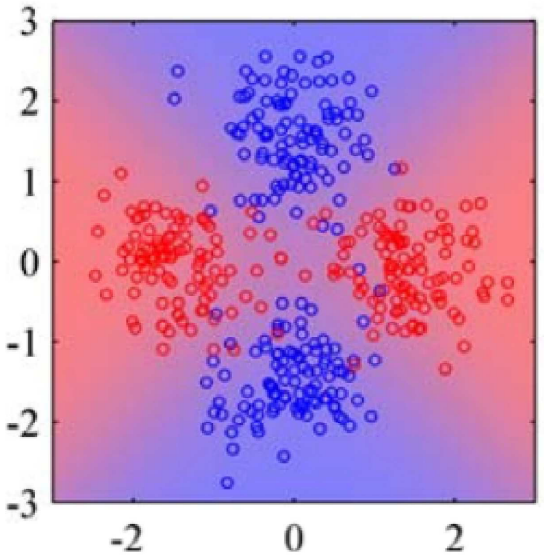

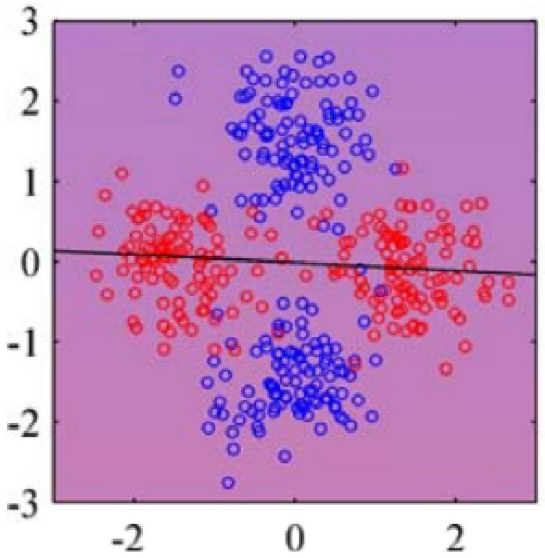

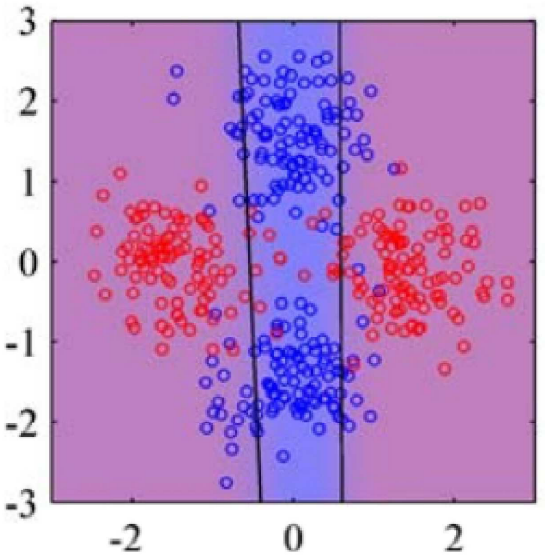

- See [Bishop 14.5.2] for more details.

Mixture of Experts : definition

- The fact that pre-estimates are functions of $\mathbf{x}$ is not exploited in the previous model.

- Mixtures of experts generalize this model by making mixing weights input-dependent :

$$\pi_k(\mathbf{x}) = \operatorname{smax}\left(\mathbf{V}^T \cdot \mathbf{x}\right).$$

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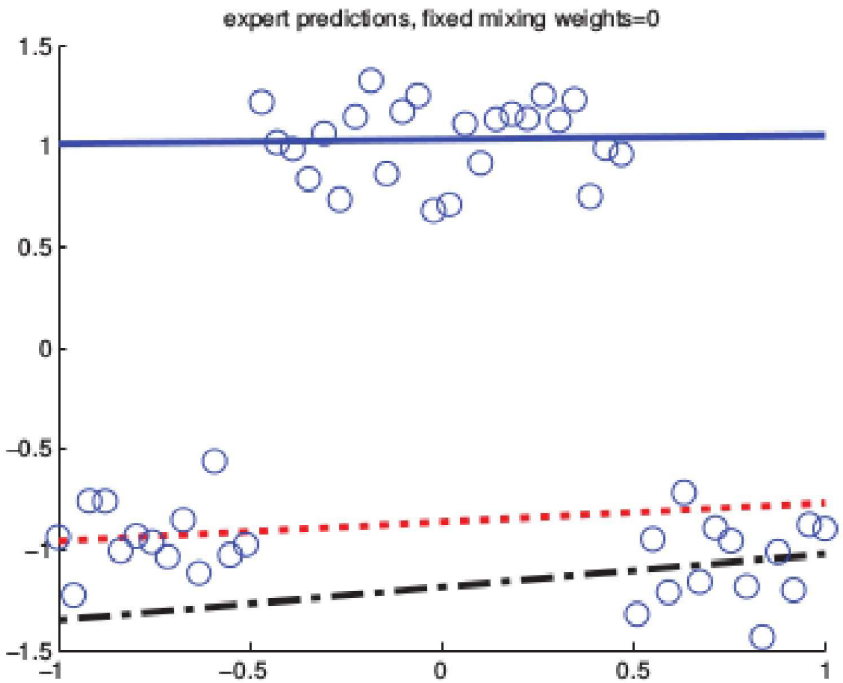
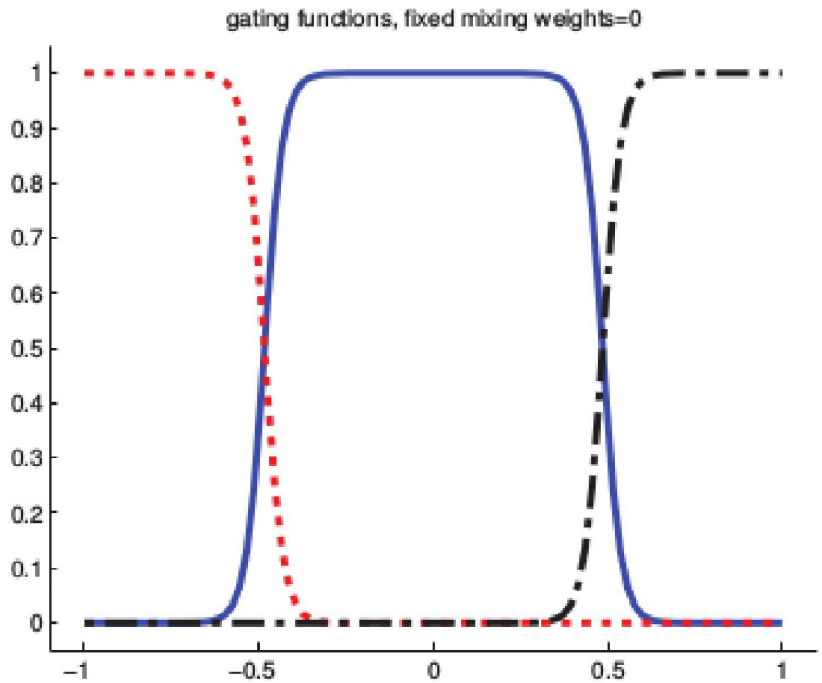
- Obviously, a linear regression is a good model for subsets of the following data :





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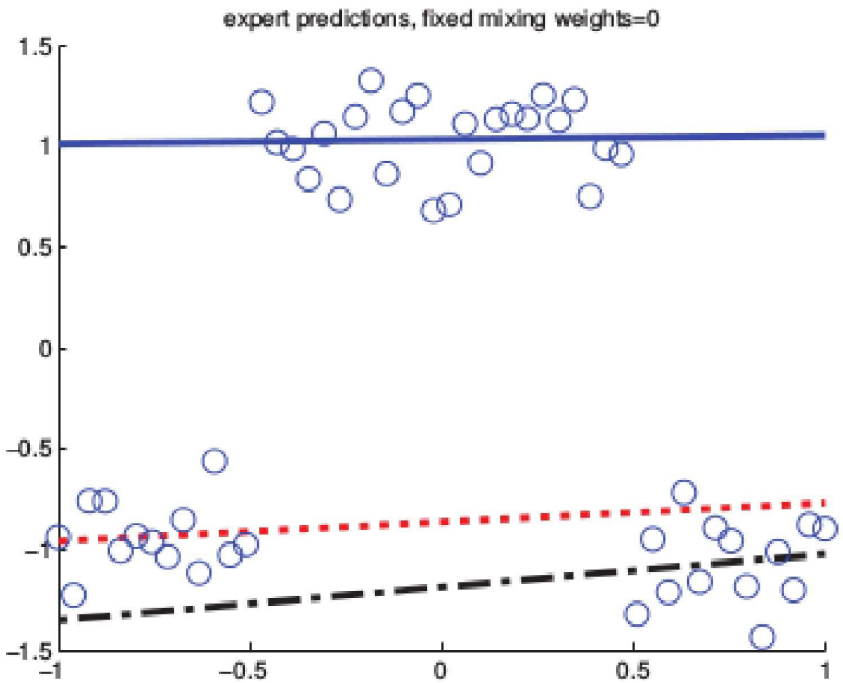

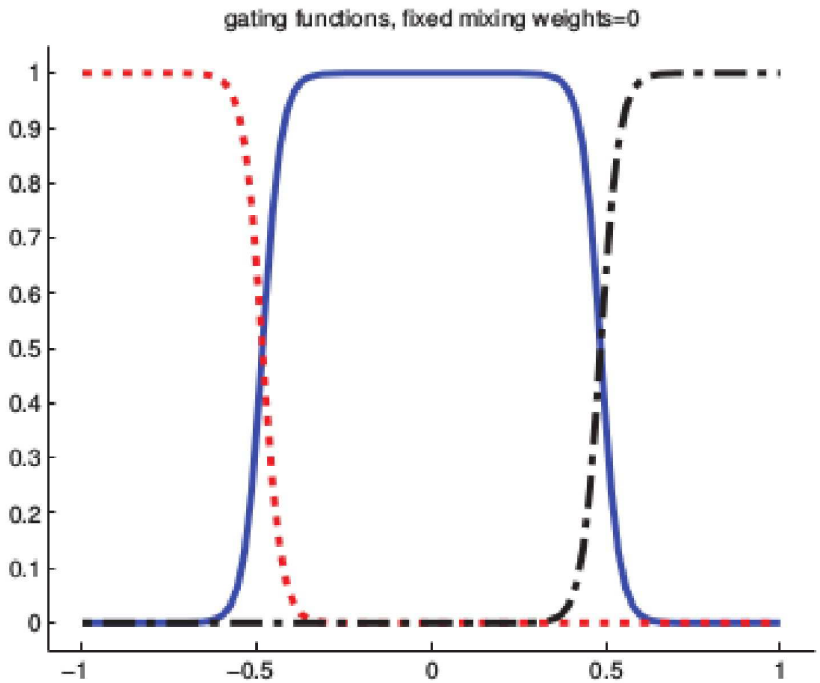

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- E step : one can show that

$$\mathbb{E}_{z^{(1)},..,z^{(n)}}\left[\log \mathcal{L}_{\text{comp}}\left(\Theta\right)\right] = \sum_{i=1}^{n}\sum_{k=1}^{2}\gamma_k^{(i)}\left[\log\left(\pi_k^{(i)}\right) - \frac{\left(y^{(i)} - \theta_k^T \cdot \mathbf{x}^{(i)}\right)^2}{2\sigma_k^2}\right],$$

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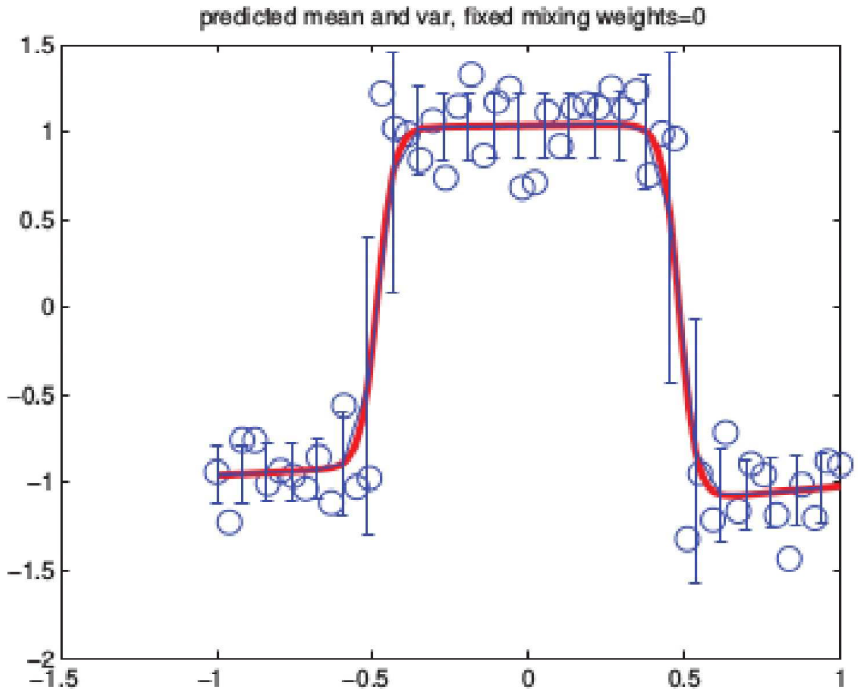

- See [Murphy 2012 - 11.4.3] for more details.

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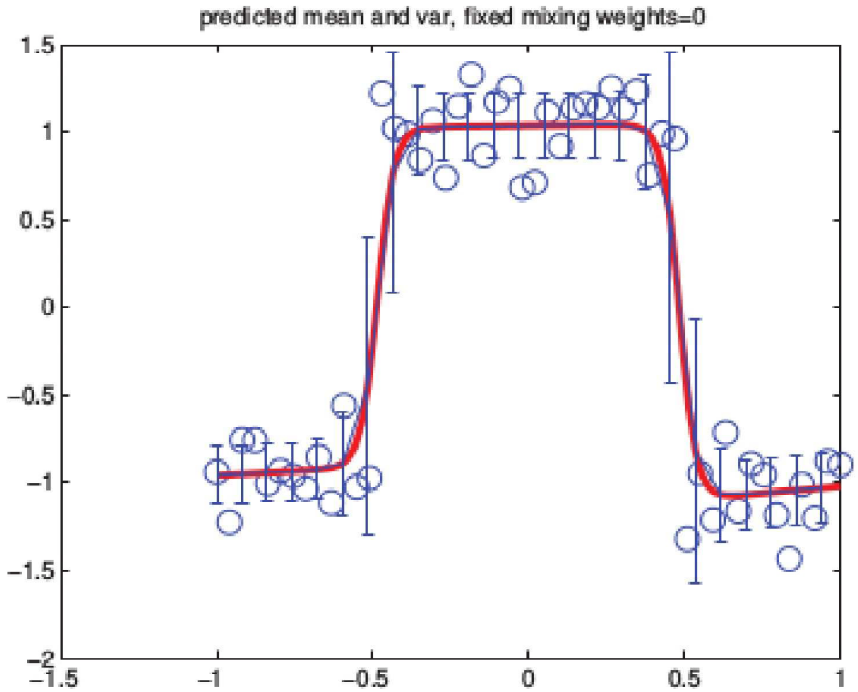

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Chapter organization

Ensemble methods : definition

- Ensemble methods are homogeneous classifier combination methods.

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1. Generate a dataset $\mathcal{D}_{\text{boot}}$ from $\mathcal{D}_{\text{train}}$ (unif. samping with replacement).
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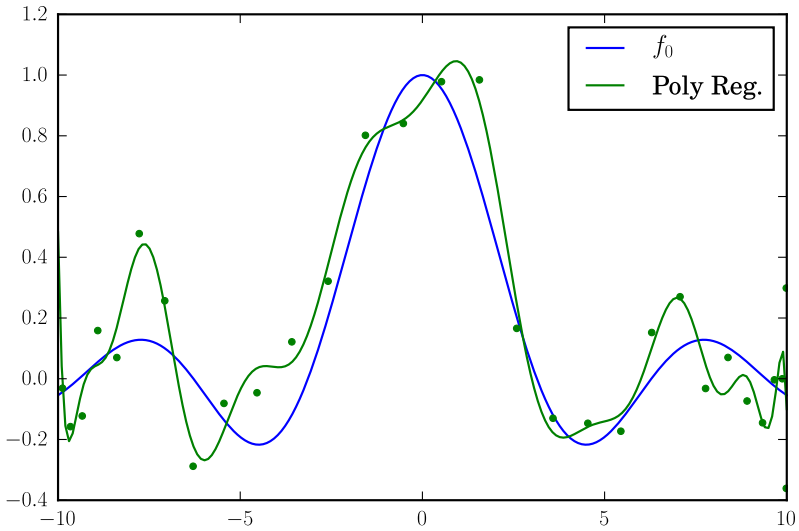
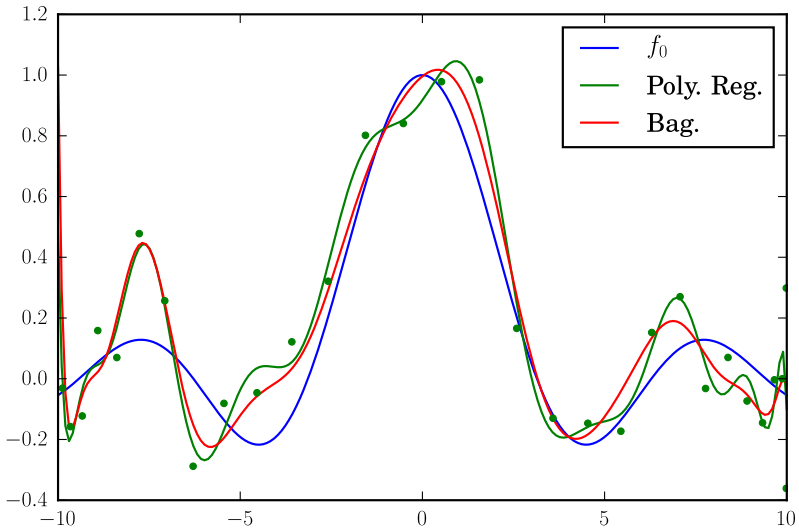
Ensemble methods : bagging - Regression example

- Suppose one fits a 20 degree polynomial on this noisy data :



Ensemble methods : bagging - Regression example

- Bagging will help a bit to mitigate overfitting



Ensemble methods : bagging - Why should it work ?

- Let ϵ_k denote the (signed) error function between the true function f_0 and one of my pre-estimate f_k that was trained on a bootstrap sample :

$$\epsilon_k(\mathbf{x}) = f_k(\mathbf{x}) - f_0(\mathbf{x}).$$

- For regression problems, the usual loss function is the **quadratic** one.

- The expected loss for the predictor $f_k(\mathbf{x})$ is thus :

$$E_{\text{out}}^{(k)} = \mathbb{E}_X\left[(f_k(\mathbf{x}) - f_0(\mathbf{x}))^2\right] = \mathbb{E}_X\left[\epsilon_k(\mathbf{x})^2\right]$$

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1. Train classifier f_k on the weighted training set $\mathcal{D}_{\text{train}} \times \left\{ w_k^{(1)}, \ldots, w_k^{(n)} \right\}$.
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- Boosting aims at minimizing a weighted **0-1 loss** over the training set :

$$J_k = \sum_{i=1}^{n} w_k^{(i)} \left(1 - \mathbb{I}_{y^{(i)}} \left(f_k \left(\mathbf{x}^{(i)}\right)\right)\right).$$

- The boosted ensemble, however, minimizes the exponential loss :

$$J_{\text{ens}} = \sum_{i=1}^{n} \exp\left(-y^{(i)} \frac{1}{2} \sum_{k=1}^{m} \alpha_k f_k \left(\mathbf{x}^{(i)}\right)\right).$$

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- Weight update :

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Ensemble methods : boosting

After f_{m+1} is learned :

- Mixing coefficients update according to

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Ensemble methods : boosting

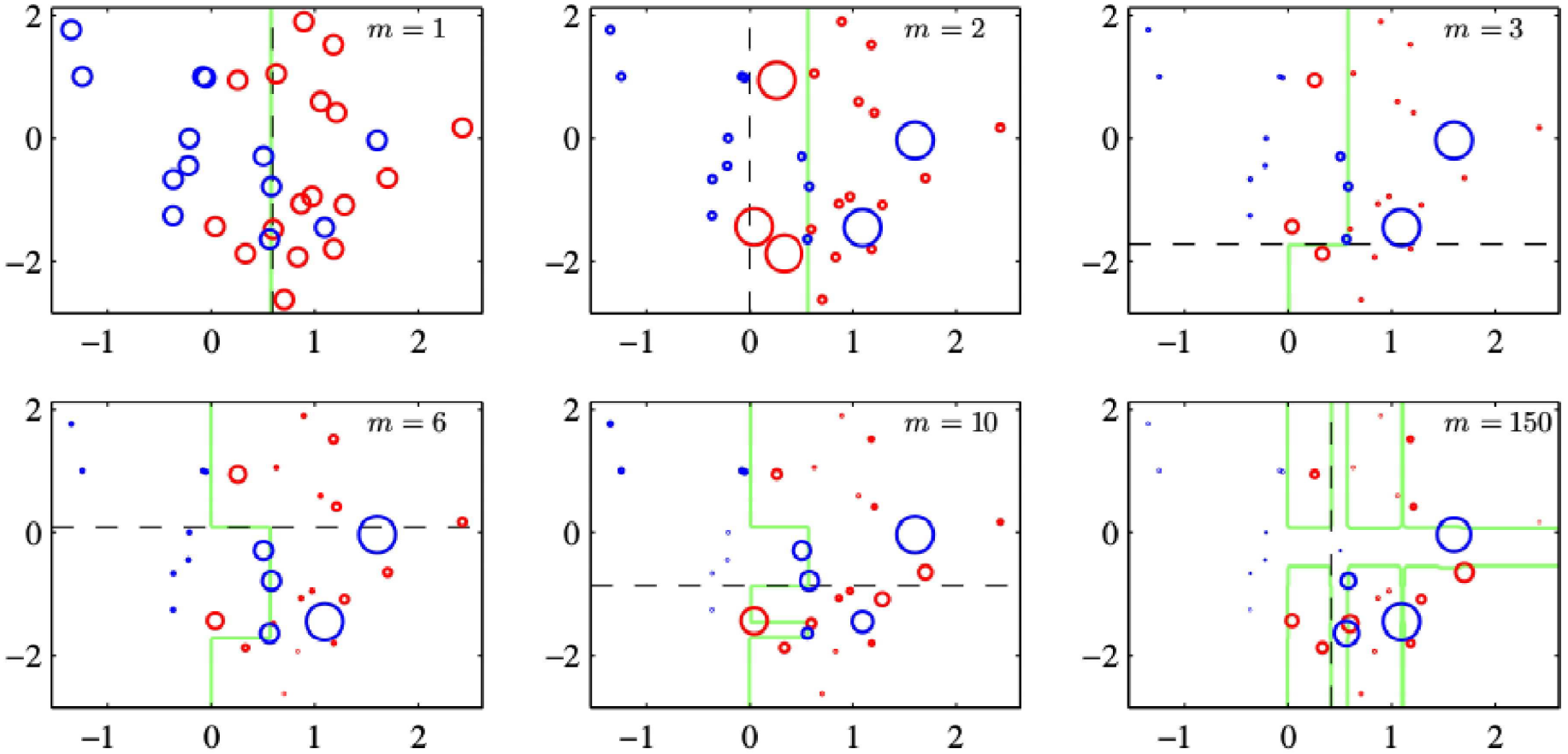
All of this essentially comes from the following decomposition of the ensemble loss :

- Denote $\mathcal{M}$ the set of misclassified points by f_{m+1}.
- Denote $\mathcal{T}$ the set of correctly classified points by f_{m+1}.
- We have

$$J_{\text{ens}} = e^{\frac{-\alpha_{m+1}}{2}} \sum_{i \in \mathcal{T}} w_{m+1}^{(i)} + e^{\frac{\alpha_{m+1}}{2}} \sum_{i \in \mathcal{M}} w_{m+1}^{(i)},$$

$$= e^{\frac{-\alpha_{m+1}}{2}} \sum_{i=1}^{n} w_{m+1}^{(i)} + \left(e^{\frac{\alpha_{m+1}}{2}} - e^{\frac{-\alpha_{m+1}}{2}} \right) \sum_{i=1}^{n} w_{m+1}^{(i)} \times \mathbb{I}\left(f_{m+1}\left(\mathbf{x}^{(i)}\right) \neq y^{(i)} \right).$$

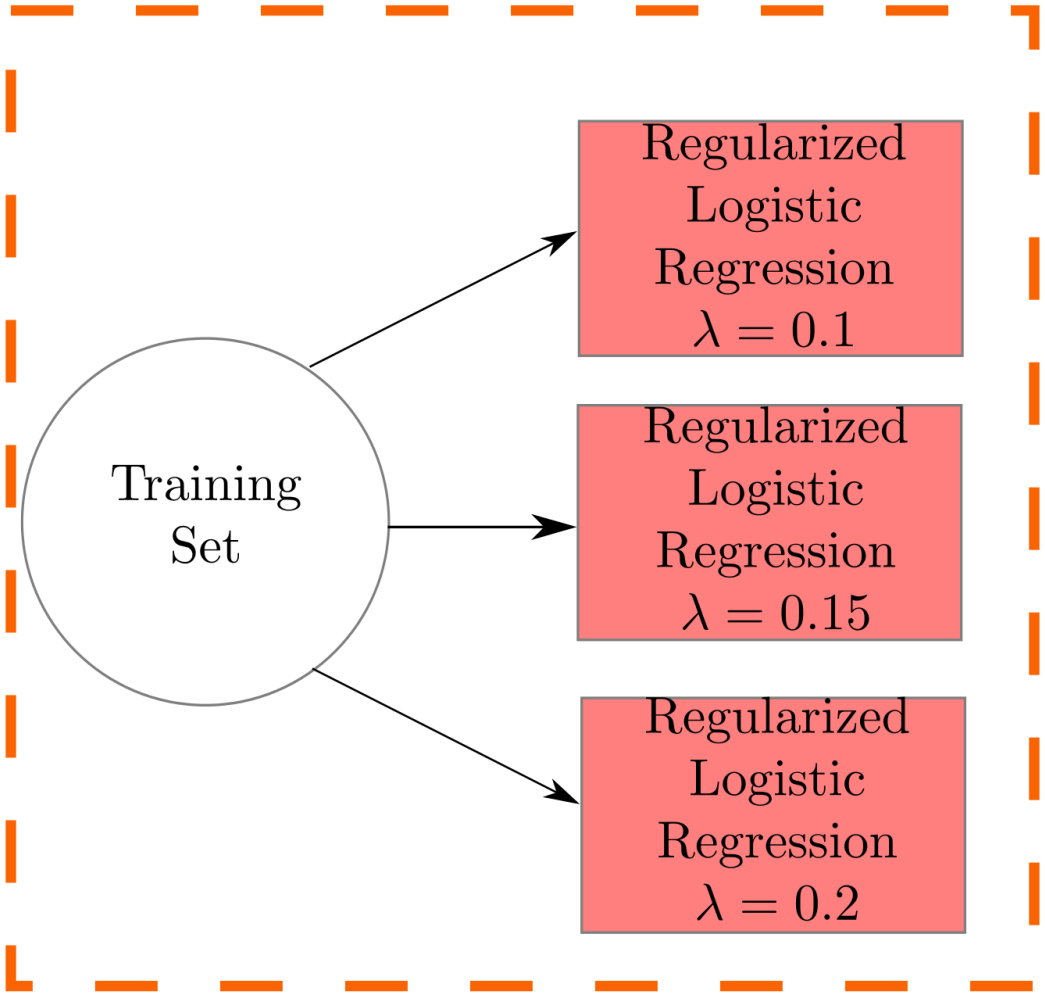
Ensemble methods : boosting - Illustration



[Bishop 2006]

Ensemble methods : stacking - Procedure

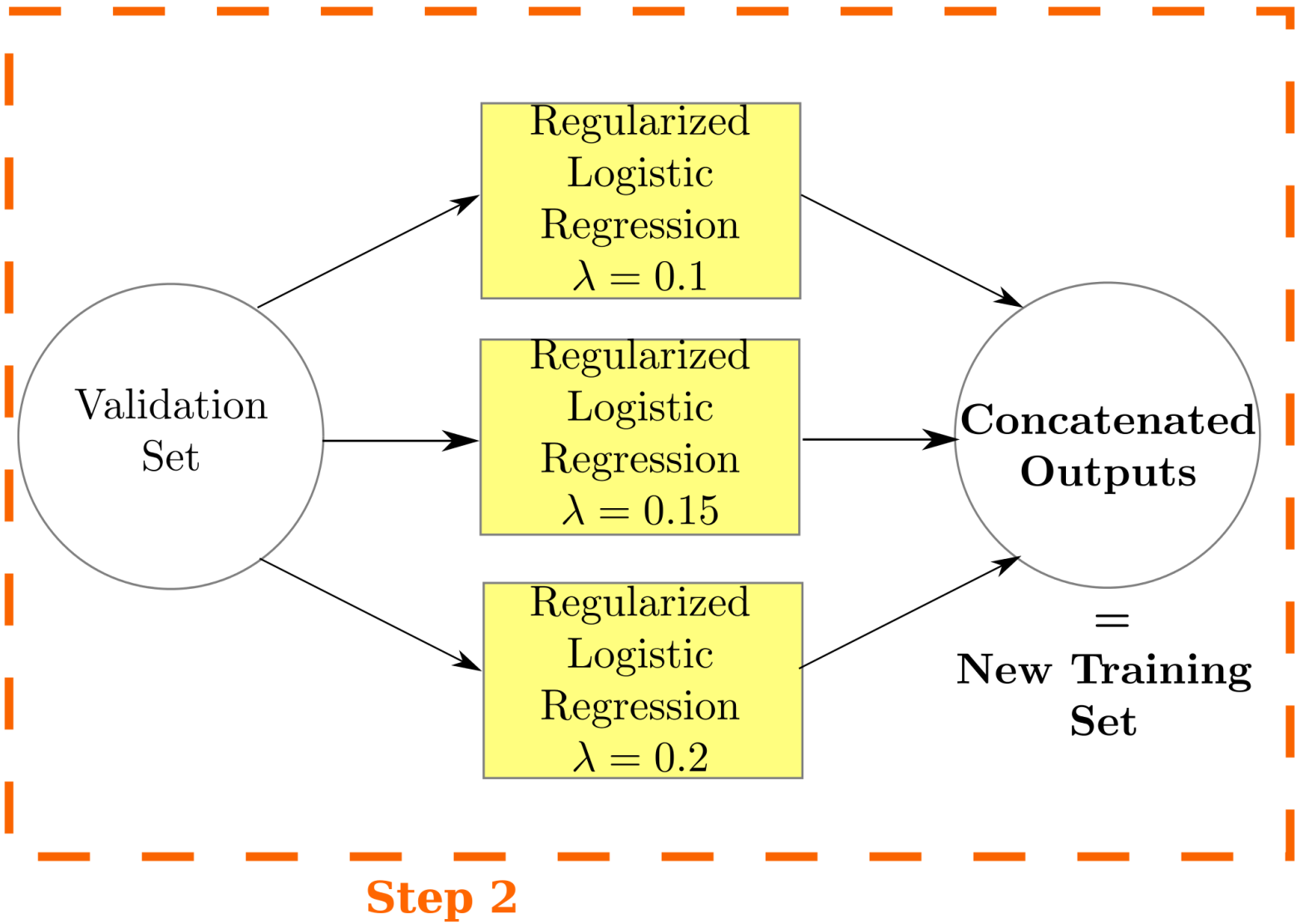
Train each member of the ensemble.



Step 1

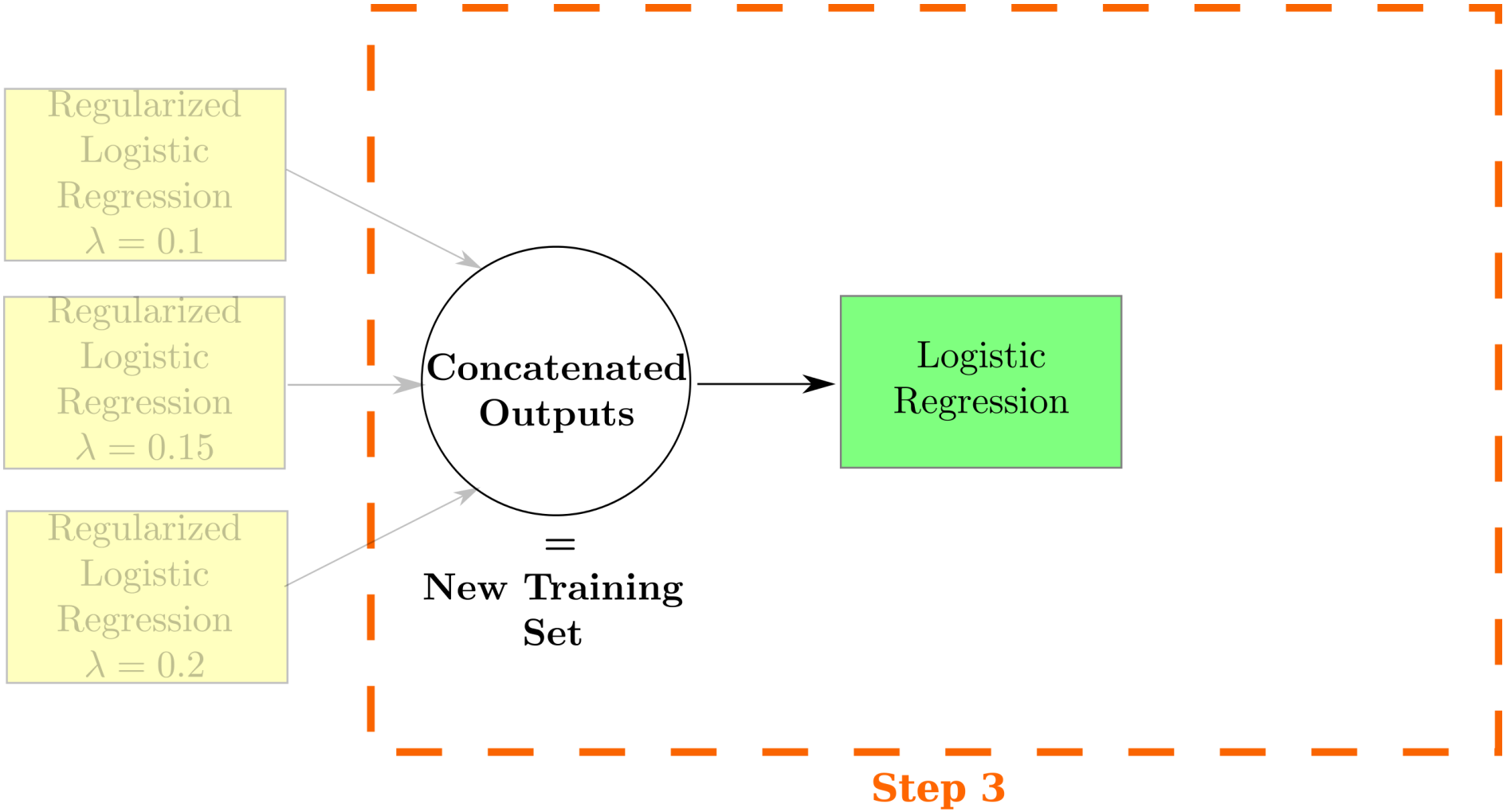
Ensemble methods : stacking - Procedure

Generate a new training set for the fusion op.



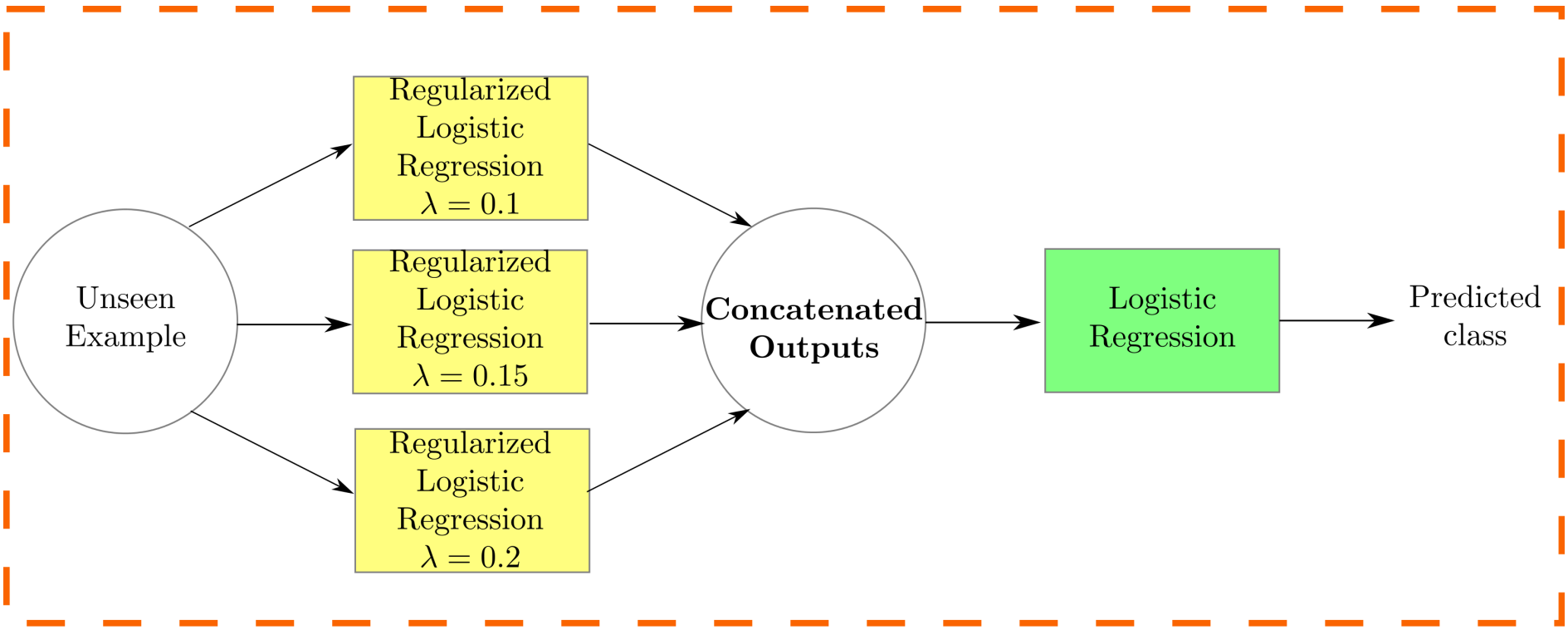
Ensemble methods : stacking - Procedure

Train the fusion op.



Ensemble methods : stacking - Procedure

Use it all.



Step 4

Ensemble methods : stacking - Comments

- Stacking can be used for heterogeneous classifiers too.
- Unlike mixture models, stacking needs private data for training the fusion op.
- Solution : repeat the procedure in a cross validation (CV) fashion.
- Supposing one performs leave-one-out CV (**LOOCV**) and let $f_k^{(-i)}$ denote the k^{th} training on the whole training set **except** data point $\mathbf{x}^{(i)}$, then in step 3, one needs to minimize

$$J(\mathbf{w}) = \sum_{i=1}^{n} L\left(y^{(i)}, \operatorname{sgm}\left(\sum_{k=1}^{m} w_k f_k^{(-i)}\right)\right).$$

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Ensemble methods : Error-correcting output codes

- Suppose examples **x** need to be sorted into $\ell > 2$ classes.
- One can assign a code encoded as a bit-vector **b** for each class.
- For example in a binary setting :

Class	b_1	b_2	b_3	b_4	b_5
a	-1	$+1$	-1	$+1$	$+1$
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- In this encryption, 0 means that the corresponding class is discarded for this binary classifier at training time.
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- Hamming distance between codes = nbr. of unequal bits
- The minimal Hamming distance between each pair of codes need to be high.
- 1 vs all scheme : each column b_i is "on" for class y_i and "off" otherwise.
- Random scheme : generate many columns s.t. each element has prob. $\frac{1}{2}$ to be $+1$ or -1. Select $10 \log \ell$ columns maximizing the minimal Hamming distance.

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- $\mathcal{Y}$ is the set of classes.
- $\text{code}^{(i)}$ is the code of class number i.
- $\text{code}(\mathbf{x})$ is the code returned by the ensemble for example $\mathbf{x}$.
- Hamming distance :

$$f^{(\text{ens})}(\mathbf{x}) = \underset{y_i \in \mathcal{Y}}{\arg\min} \; d_{\text{ham}}\left(\text{code}^{(i)}, \text{code}(\mathbf{x})\right).$$

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Chapter organization

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- A catch sentence for this chapter could be :

  « Why use only one classifier when I can use many ? »

- With Bayesian learning, this would become :

  « Why use only one classifier when I can use infinitely many ? »

- Let us see under which circumstances such a result can be achieved.

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Bayesian Learning : - starting point

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$$\arg\min_{\boldsymbol{\theta}} \quad \mathrm{DataFit}\left(\boldsymbol{\theta}\right) \quad + \quad \mathrm{Regularizer}\left(\boldsymbol{\theta}\right).$$

- In this setting, each $f \in \mathcal{H}$ is in bijective correspondence with a given $\theta \in \Theta$.

- Almost all such algorithms have an equivalent probabilistic formulation :

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- Suppose we are trying to predict the selling price y of a house.
- For each house, we collected data like surface, previous buying price, GPS coordinates, etc.
- These features are concatenated into a vector $\mathbf{x}$;
- We need to learn the function f_0 mapping vectors $\mathbf{x}$ to y.
- We believe a linear combination of the features should be a relevant model :

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$$Y \sim \mathcal{N}\left(\boldsymbol{\theta}^T \cdot \mathbf{x}, \sigma\right).$$

- Now the likelihood is given by :

$$\text{Likelihood}\left(\theta\right) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{\left(y^{(i)} - \theta^T \cdot \mathbf{x}^{(i)}\right)^2}{2\sigma^2}}$$

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- We already have some knowledge on what values of $\boldsymbol{\theta}$ are more likely before seeing any datum :

$$\text{Prior}\left(\boldsymbol{\theta}\right) = \frac{1}{\left(2\pi\right)^{\frac{d}{2}} \det\left(\mathbf{V}_0\right)^{\frac{1}{2}}} e^{-\frac{1}{2}\left(\boldsymbol{\theta}-\boldsymbol{\theta}_0\right)^T \cdot \mathbf{V}_0^{-1}\left(\boldsymbol{\theta}-\boldsymbol{\theta}_0\right)}$$

- After seeing data $\mathcal{D}$, our knowledge is given by the following posterior distribution

$$p\left(\boldsymbol{\theta}|\mathcal{D}, \boldsymbol{\theta}_0, \mathbf{V}_0\right) \quad \propto \quad \text{Likelihood}\left(\boldsymbol{\theta}\right) \quad \times \quad \text{Prior}\left(\boldsymbol{\theta}\right).$$

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Bayesian Learning : - Linear regression example

- If the prior parameters are such that $\boldsymbol{\theta}_0 = \mathbf{0}$ and $\mathbf{V}_0 = \tau^2 \mathbf{I}$, applying
  – log leads to the following cost function (up to an additive constant)

$$J(\boldsymbol{\theta}) = \underbrace{\sum_{i=1}^{n} \frac{\left(y^{(i)} - \boldsymbol{\theta}^T \cdot \mathbf{x}^{(i)}\right)^2}{2\sigma^2}}_{\text{Least Squares}} + \underbrace{\frac{1}{\tau^2} \|\boldsymbol{\theta}\|_2}_{\text{Ridge Reg.}}$$

Bayesian Learning : - Linear regression example

- Going back to probabilities, one can show that the posterior $p(\boldsymbol{\theta}|\mathcal{D}, \boldsymbol{\theta}_0, \mathbf{V}_0)$ is also Gaussian, in which case our prior is conjugate[2].

$$p(\boldsymbol{\theta}|\mathcal{D}, \boldsymbol{\theta}_0, \mathbf{V}_0) \sim \mathcal{N}(\boldsymbol{\theta}_n, \mathbf{V}_n), \tag{3}$$

$$\boldsymbol{\theta}_n = \mathbf{V}_n \left(\mathbf{V}_0^{-1} \cdot \boldsymbol{\theta}_0 + \frac{1}{\sigma^2} \mathbf{X}^T \cdot \mathbf{y} \right), \tag{4}$$

$$\mathbf{V}_n = \left(\mathbf{V}_0^{-1} + \frac{1}{\sigma^2} \mathbf{X}^T \cdot \mathbf{X} \right)^{-1}, \tag{5}$$

with

$$\mathbf{X} = \begin{pmatrix} — \left(\mathbf{x}^{(1)}\right)^T — \\ \vdots \\ — \left(\mathbf{x}^{(n)}\right)^T — \end{pmatrix} \quad \text{and} \quad \mathbf{y} = \begin{pmatrix} y^{(1)} \\ \vdots \\ y^{(n)} \end{pmatrix}.$$

2. Under conjugacy, learning boils down to updating the prior parameters and the updates are easy to compute.

Bayesian Learning : - Linear regression example

- No fusion for now .. just Bayesian statistics !

- As learners, what we really need is the posterior predictive $p(y|\mathbf{x}, \mathcal{D})$.

- The expectation of this distribution is our proxy for f_0 and allows to make a prediction for the selling price of a house whose features are the entries of the unseen example $\mathbf{x}$.

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Bayesian Learning : - Linear regression example

- Observe that the predictive distribution is free of un-observed parameter conditioning... because we marginalized them out :

$$p\left(y|\mathbf{x},\mathcal{D}\right) = \int_{\Theta} p\left(y|\mathbf{x},\mathcal{D},\boldsymbol{\theta}\right) p\left(\boldsymbol{\theta}|\mathbf{x},\mathcal{D}\right) d\boldsymbol{\theta} \tag{6}$$

- The above calculus is the weighted combination of an infinity of regressors !

- The weights depend on the ability of each regressor to fit well the data.

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- In our linear regression case, we have

$$p(y|\mathbf{x},\mathcal{D}) = \int_{\Theta} p(y|\mathbf{x},\mathcal{D},\boldsymbol{\theta})\, p(\boldsymbol{\theta}|\mathbf{x},\mathcal{D})\, d\boldsymbol{\theta}, \quad (7)$$

$$= \int_{\Theta} p(y|\mathbf{x},\mathcal{D},\boldsymbol{\theta})\, p(\boldsymbol{\theta}|\mathcal{D})\, d\boldsymbol{\theta}, \quad (8)$$

$$= \int_{\Theta} G\left(y; \boldsymbol{\theta}^T \cdot \mathbf{x}, \sigma^2\right) G(\boldsymbol{\theta}; \boldsymbol{\theta}_n, \mathbf{V}_n)\, d\boldsymbol{\theta}, \quad (9)$$

with G the Gaussian density function.

- Finally, one can show that

$$y|\mathbf{x},\mathcal{D} \sim \mathcal{N}\left(\boldsymbol{\theta}_n^T \cdot \mathbf{x}, \sigma_n\right), \quad (10)$$

$$\sigma_n^2 = \sigma^2 + \mathbf{x}^T \cdot \mathbf{V}_n \cdot \mathbf{x}. \quad (11)$$

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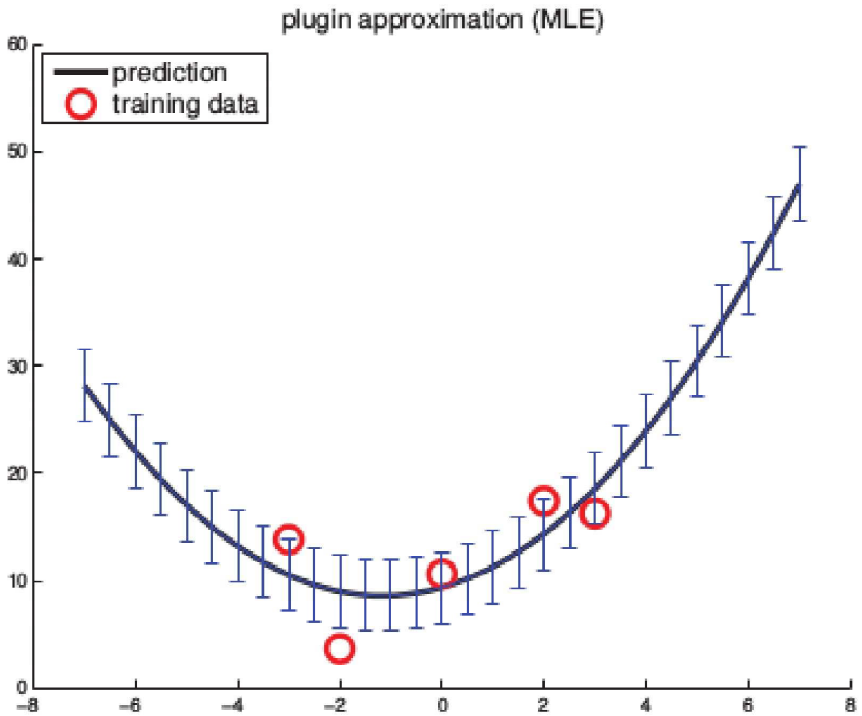
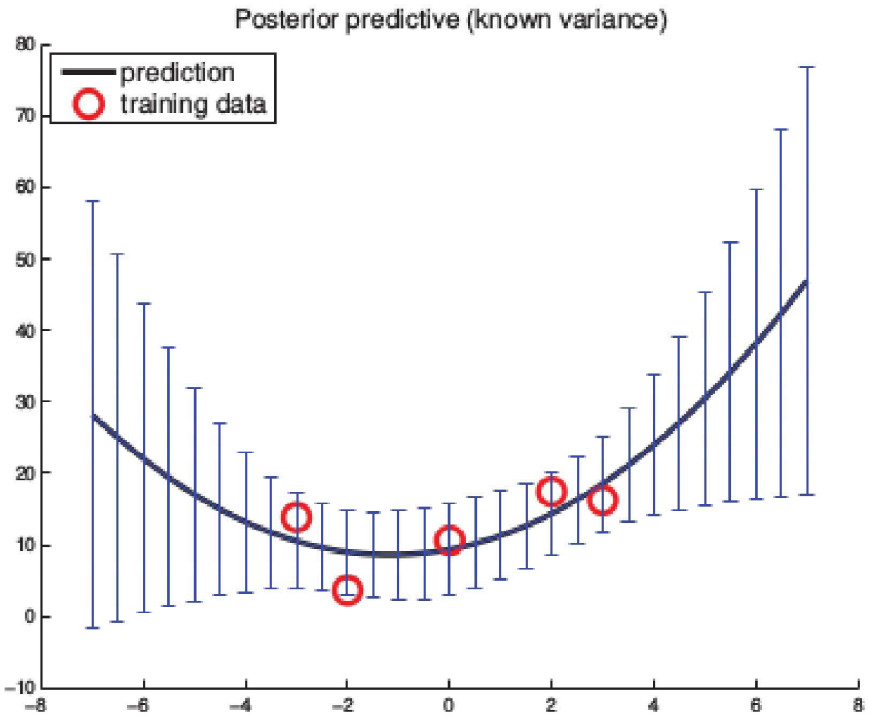
Bayesian Learning : - Illustration (polynomial reg.)





[Murphy 2012 - 7.6]

Bayesian Learning : - Comments

- The posterior predictive is not always known in closed form $\longrightarrow$ use Monte-Carlo to approximate the marginalization.
- Have we really gotten rid of all the parameters ?
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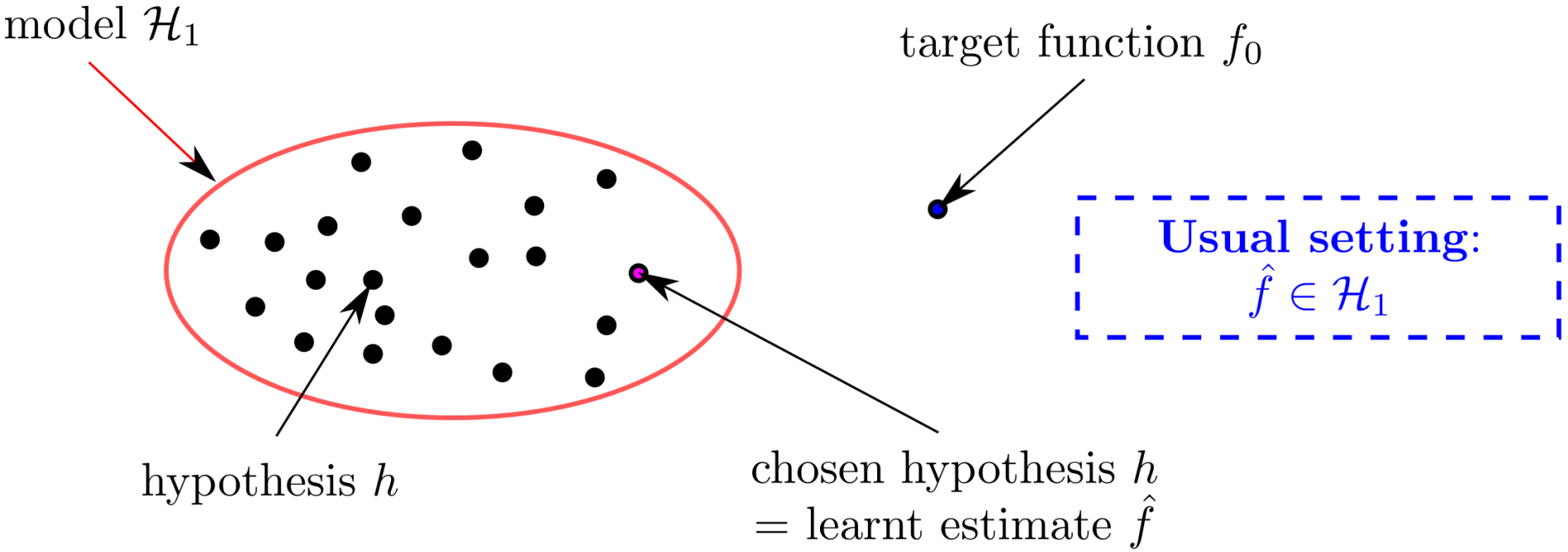
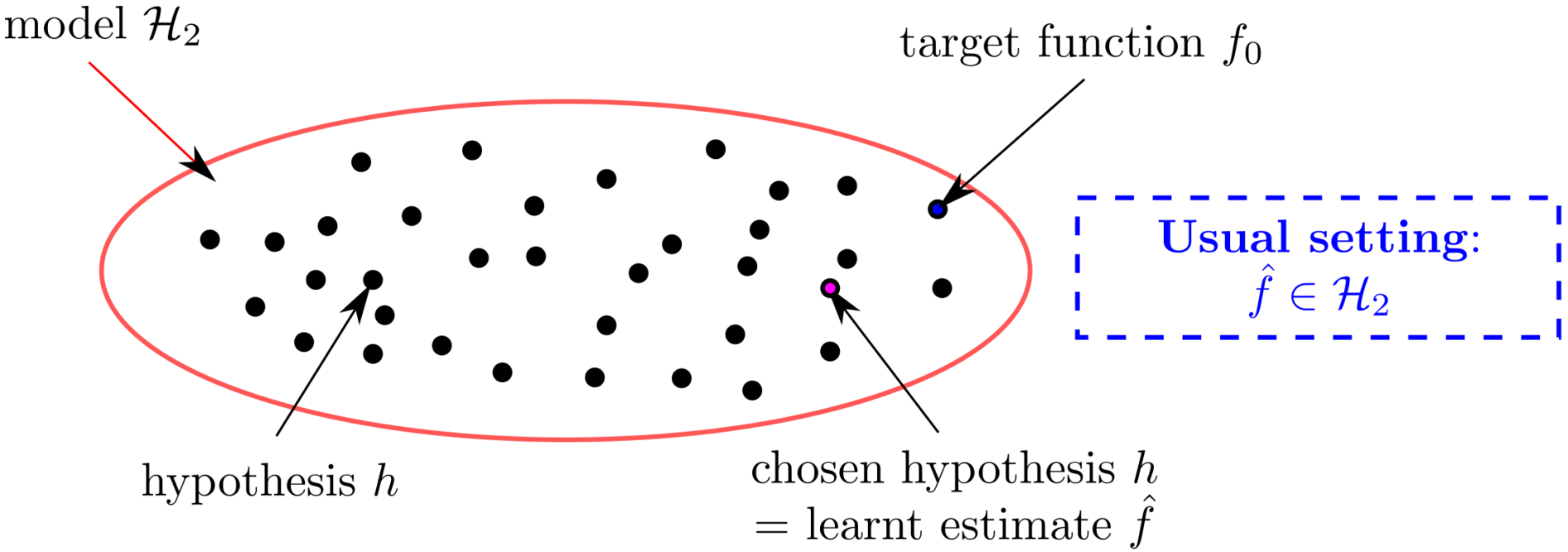
Bayesian Model Averaging : let's start with model selection

Example : Polynomial regression with small degree $q = 1$



Bayesian Model Averaging : let's start with model selection

Example : Polynomial regression with higher degree $q = 2$



Usual setting:
$\hat{f} \in \mathcal{H}_2$

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Bayesian Model Averaging : comments

- BMA only works for probabilistic models allowing to determine both $p(q|\mathcal{D})$ and $p(y|\mathbf{x}, \mathcal{D}, q)$.
- Its philosophy is close to hierarchical Bayes in the sense that each hyperprior parameter choice can be regarded as a given model.
- Difference with a mixture model :

Mixture Model	BMA
1 model	Many models and one of them is the good one
The data is explained by multiple components	The data is explained by one of the model (This model might be itself a mixture model.)

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Chapter organization

Statistical aggregation theory :

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Statistical aggregation theory : problem statement

- For simplicity, suppose the hypothesis set [3] $\mathcal{H}$ is finite : $|\mathcal{H}| = m < \infty$.
- Let $\mathcal{H}_\Theta$ denote the following space :

$$\mathcal{H}_\Theta = \left\{ f_\theta = \sum_{j=1}^{m} \theta_j f_j : \theta \in \Theta \right\}.$$

- $\mathcal{H}_\Theta$ is the functional vector space spanned by the members of $\mathcal{H}$.

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Depending the $\Theta \subseteq \mathbb{R}^m$, several sub-classes of problems are obtained :

- **Model selection** : Θ is the set of canonical base vectors, or one-hot vectors.

$$\boldsymbol{\theta}^T = \begin{bmatrix} 0 & \dots & 0 & 1 & 0 & \dots & 0 \end{bmatrix}$$

- Convex aggregation : Θ is the canonical simplex of $\mathbb{R}^m$,

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- Linear aggregation : $\Theta = \mathbb{R}^m$.

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Let $R(f_\theta)$ denote the expected loss (risk) of the pre-estimator f_θ :

$$R(f_\theta) = \mathbb{E}_{X,Y}\left[L\left(f_\theta(\mathbf{x}), y\right)\right].$$

Definition

$\theta^\star$ is an **oracle** for the aggregation problem if

$$R(f_{\theta^\star}) = \inf_{\theta \in \Theta} R(f_\theta).$$

Statistical aggregation theory : problem statement

What are we looking for ?

- An aggregated estimate $\hat{\theta}$ close to the oracle $\theta^{\star}$.
- An aggregated estimate $\hat{\theta}$ learnt from private data $\mathcal{D}_{\text{val}}$.

Close in what sense ?

- In a the following probabilistic sense :

$$\mathbb{E}_{\mathcal{D}_{\text{val}}}\left[R\left(f_{\hat{\theta}}\right)\right] \leq C \inf_{\theta \in \Theta} \left\{R\left(f_{\theta}\right) + \Delta_{n,m}\left(\theta\right)\right\},$$

with constant $C \geq 1$ and rate $\Delta_{n,m} \longrightarrow 0$ as $n \longrightarrow \infty$.

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- New question : for a given Θ, what is the best rate $\Delta_{n,m}$?

Definition

Let $\mathcal{F}$ denote a functional space.
Optimal rates or minimax rates are a sequence $\Phi_{n,m}$ such that

(i) For any pre-estimates $f_1, \ldots, f_m$ and any target f_0, there is an aggregate $f_{\tilde{\theta}}$ s.t.

$$R\left(f_{\tilde{\theta}}\right) - R\left(f_0\right) \leq c_1 \Phi_{n,m}$$

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Example : for linear aggregation of regressors (under additive Gaussian noise), we have

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Penalized approaches :

- Since the distribution $p_{X,Y}$ is unknown, explicit risk computation is impossible.

- A biased proxy for it is the empirical risk

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- Keep in mind that for each f_k, the training error is

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- Keep in mind that for each f_k, the training error is

$$Err_{\text{train}} = \sum_{\left(\mathbf{x}^{(i)}, y^{(i)}\right) \in \mathcal{D}_{\text{train}}} L\left(y^{(i)}, f_k\left(\mathbf{x}^{(i)}\right)\right).$$

Statistical aggregation theory : some solutions

Penalized approaches :

- A possibility to learn $\hat{\boldsymbol{\theta}}$ is to minimize the empirical risk

$$\hat{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta}} R_{\text{emp}}\left(f_{\boldsymbol{\theta}}\right).$$

- This is doomed to overfit, and therefore we solve

$$\hat{\theta} = \arg\min_{\theta} R_{\text{emp}}\left(f_{\theta}\right) + \text{Regularizer}\left(\theta\right).$$

- This penalized problem mimics the oracle bound, yet the regularizer does not depend on n !

- By carefully choosing $\text{Regularizer}\left(\theta\right)$ (with a $\|\theta\|_0$ term in it), then minimax rates are achieved for linear, convex and model selection aggregation problems.

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Statistical aggregation theory : some solutions

Exponential weights :

- In the convex aggregation problem, weights $\left[\theta_1 \dots \theta_m\right]$ can be regarded as a probability distribution.

- By choosing a regularizer involving the Kullback-Leibler divergence between θ and a prior π and by replacing the empirical risk with the surrogate

$$\sum_{j=1}^{m} \theta_k R_{\text{emp}}\left(f_k\right),$$

we obtain

$$\hat{\theta} = \operatorname{smax}\left(n \begin{bmatrix} \pi_1 R_{\text{emp}}\left(f_1\right) \\ \vdots \\ \pi_m R_{\text{emp}}\left(f_m\right) \end{bmatrix}\right).$$

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- Benjamin Guedj (INRIA / Painlevé - MODAL) homepage

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