Foundations of Machine Learning

Regression

Nov 2021

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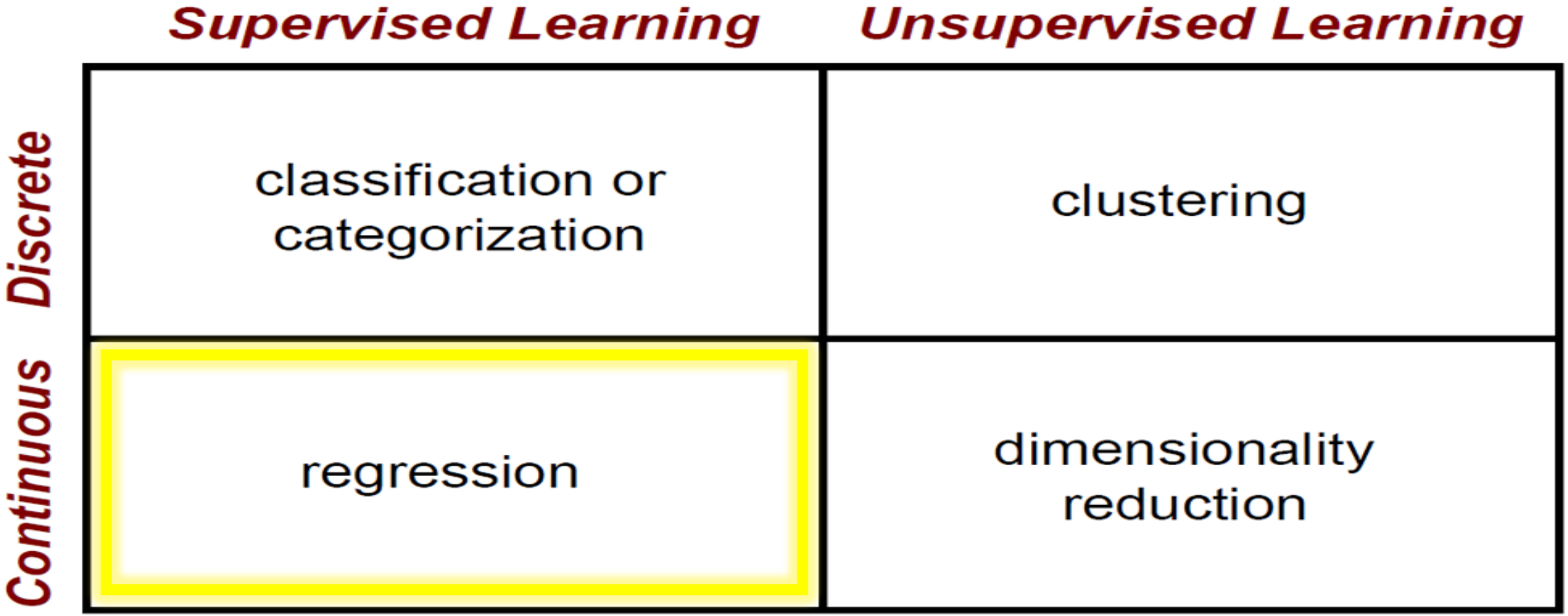
ML Problems

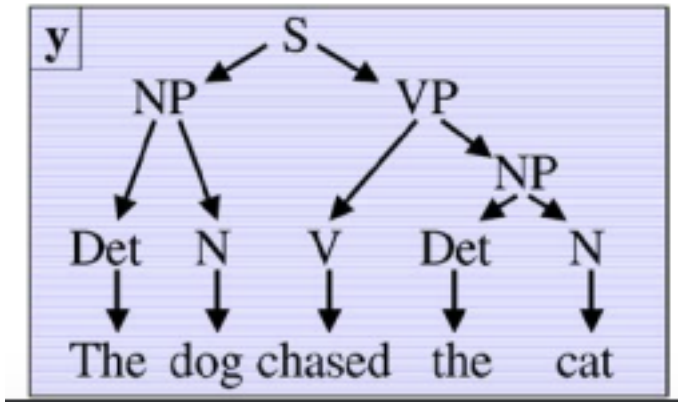

Supervised Learning
Unsupervised Learning
Discrete
Continuous
classification or categorization
clustering
regression
dimensionality reduction

Going beyond Discrete Class Labels

- So far we have focused on classification $f : X \rightarrow \{1, \ldots, k\}$

  What about other outputs?

- PM2.5 (pollutant) particulate matter exposure estimate:
  - Input: # cars, temperature, etc.
  - Output: 50 ppb
- Pose estimation:
- Sentence structure estimate:



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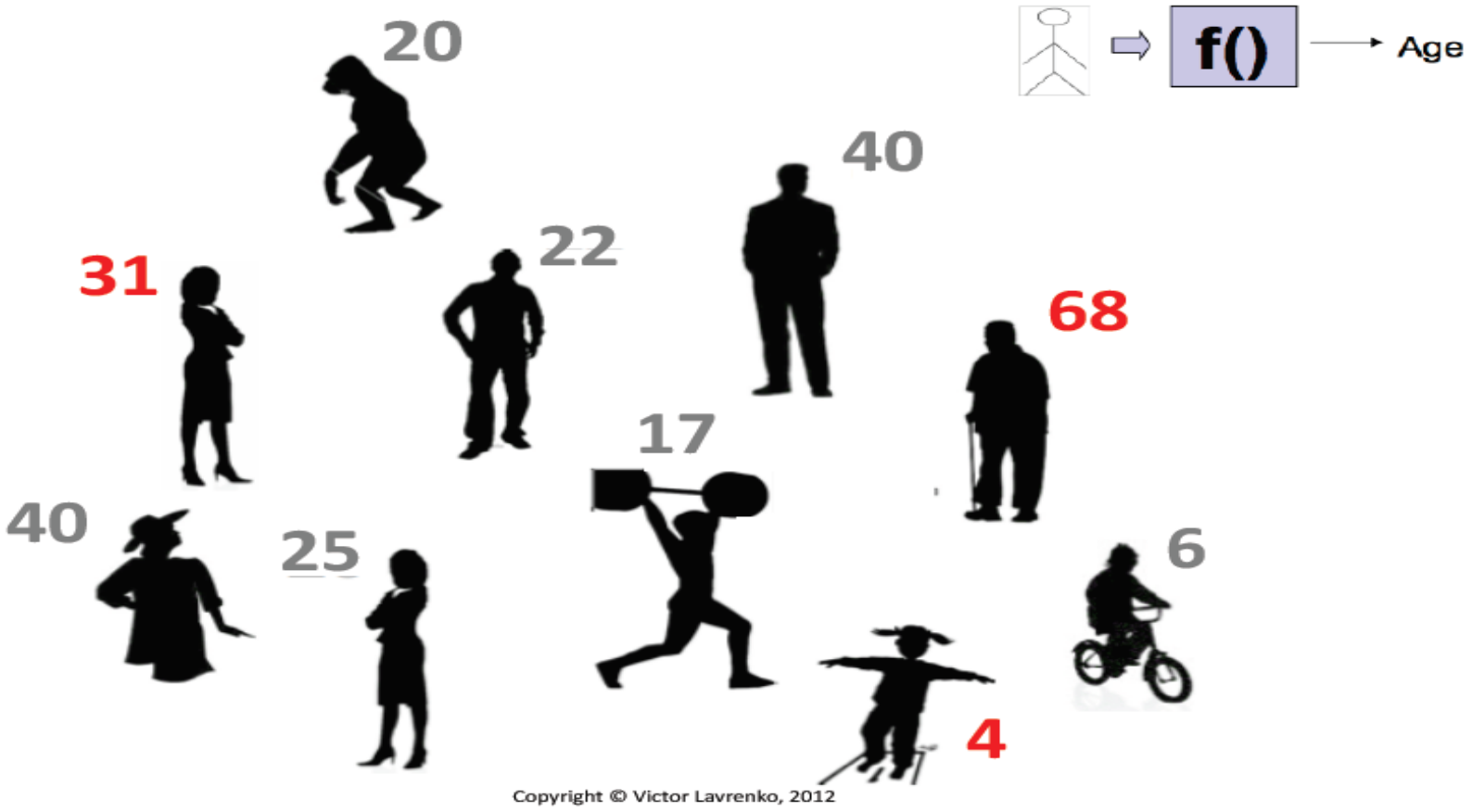
Regression (Supervised Learning)



Regression Methods

- Linear Least-Squares Regression
  - Partial Least-Squares
  - Total Least-Squares
  - Ridge Regression, LASSO
- Kernel Regression
- k-NN Regression
- Regression Trees
- Support Vector Regression
- Logistic Regression

Regression Formulation

Given x, want to predict an estimate $\hat{y}$ of y, which minizes the discrepancy (L) between $\hat{y}$ and y.

$$L(\hat{y}; y) := |\hat{y} - y| \quad \textit{Absolute error}$$

$$:= (\hat{y} - y)^2 \quad \textit{Squared error}$$

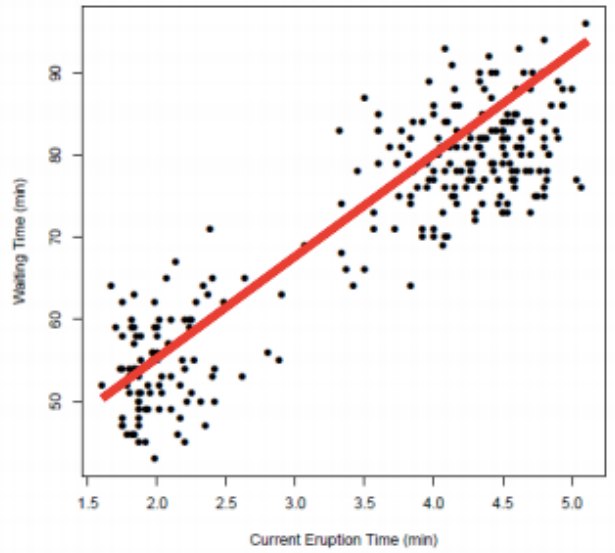
Loss

A **linear predictor** f, can be defined by the slope w and the intercept w_0 :

$$\hat{f}(\vec{x}) := \vec{w} \cdot \vec{x} + w_0$$

which minimizes the prediction loss.

$$\min_{w, w_0} \mathbb{E}_{\vec{x}, y} \left[L(\hat{f}(\vec{x}), y) \right]$$



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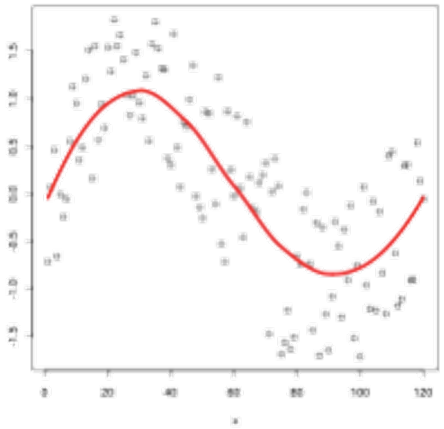
Parametric (vs) Non-parametric Regression

If we assume a particular form of the regressor:

Parametric regression

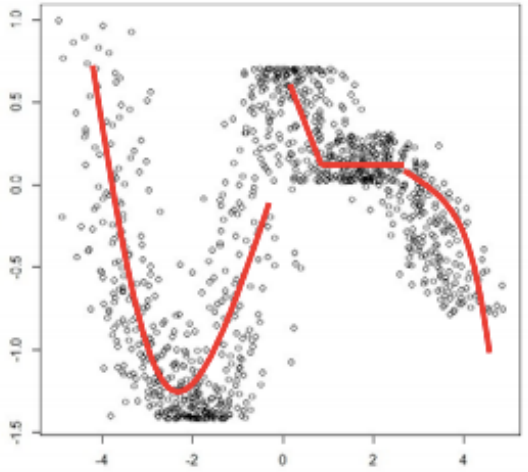
Goal: to learn the parameters which yield the minimum error/loss



If no specific form of regressor is assumed:

Non-parametric regression

Goal: to learn the predictor directly from the input data that yields the minimum error/loss



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Linear Regression

Want to find a **linear predictor** f, i.e., w (intercept w_0 absorbed via lifting):

$$\hat{f}(\vec{x}) := \vec{w} \cdot \vec{x}$$

which minimizes the prediction loss over the population.

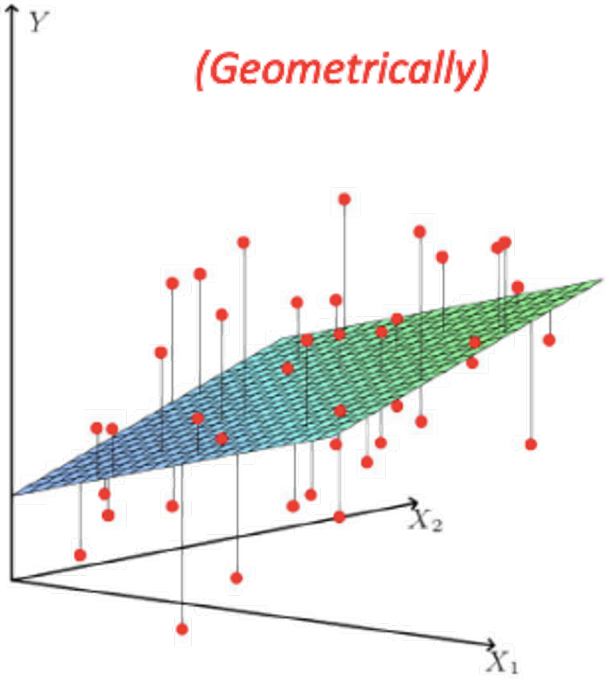
$$\min_{\vec{w}} \mathbb{E}_{\vec{x},y}\left[L(\hat{f}(\vec{x}), y)\right]$$

We estimate the parameters by minimizing the corresponding loss on the training data:

$$\arg\min_{w} \frac{1}{n}\sum_{i=1}^{n}\left[L(\vec{w}\cdot\vec{x}_i, y_i)\right]$$

$$= \arg\min_{w} \frac{1}{n}\sum_{i=1}^{n}\left(\vec{w}\cdot\vec{x}_i - y_i\right)^2$$

for squared error



(Geometrically)

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Linear Regression

Linear predictor with squared loss:

$$\arg\min_{w} \frac{1}{n} \sum_{i=1}^{n} \left(\vec{w} \cdot \vec{x}_i - y_i\right)^2$$

$$= \arg\min_{w} \left\| \begin{pmatrix} \dots x_1 \dots \\ \dots x_i \dots \\ \dots x_n \dots \end{pmatrix} \begin{pmatrix} w \end{pmatrix} - \begin{pmatrix} y_1 \\ y_i \\ y_n \end{pmatrix} \right\|^2$$

$$= \arg\min_{w} \left\| X\vec{w} - \vec{y} \right\|_2^2$$

Unconstrained problem!

Can take the gradient and examine the stationary points!

Why need not check the second order conditions?

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Linear Regression

Best fitting *w*:

$$\frac{\partial}{\partial \vec{w}} \|X\vec{w} - \vec{y}\|^2 = 2X^\top (X\vec{w} - \vec{y})$$

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

At a stationary point

$$\implies \vec{w}_{\text{ols}} = (X^\top X)^\dagger X^\top \vec{y}$$

Pseudo-inverse

Also called the Ordinary Least Squares (OLS)

The solution is unique and stable when X^TX is invertible

What is the interpretation of this solution?

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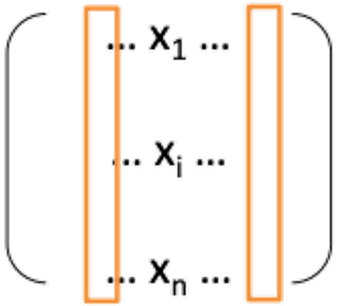
Linear Regression: Geometric Interpretation

Consider the ***column space*** view of data **X**:



$$\ddot{x}_1, \ldots, \ddot{x}_d \in \mathbf{R}^n$$

Find a *w*, such that the linear combination of ***minimizes***

$$\frac{1}{n}\left\|\vec{y} - \sum_{i=1}^{d} w_i \ddot{x}_i\right\|^2 =: \text{residual}$$

$$\hat{y} = X\vec{w}_{\text{ols}} = X(X^\top X)^\dagger X^\top \vec{y}$$

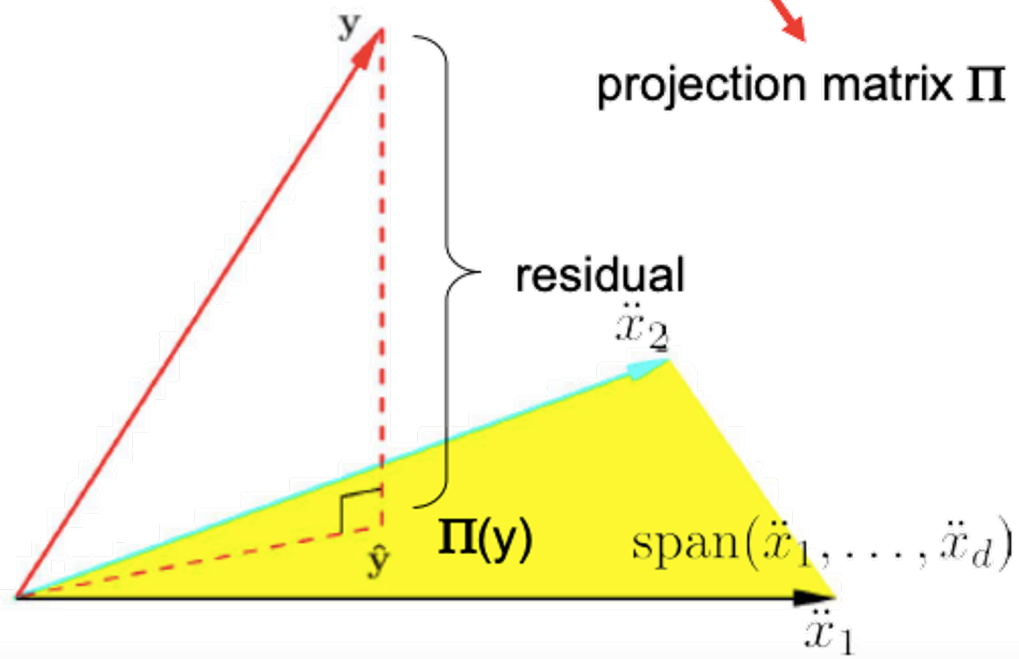
projection matrix $\mathbf{\Pi}$

Say $\hat{y}$ is the ols solution, ie,

$$\hat{y} := X\vec{w}_{\text{ols}} = \sum_{i=1}^{d} w_{\text{ols},i}\ddot{x}_i$$

*Thus, $\hat{y}$ is the **orthogonal projection** of y onto the $\text{span}(\ddot{x}_1, \ldots, \ddot{x}_d)$!*

*w_{ols} forms the **coefficients** of $\hat{y}$*



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Linear Regresssion: Statistical Modeling View

Let's assume that data is **generated** from the following process:

- A example x_i is draw independently from the data space **X**

$$x_i \sim \mathcal{D}_X$$

- y_{clean} is computed as $(w \,.\, x_i)$, from a fixed unknown w

$$y_{\text{clean}} := w \cdot x_i$$

- y_{clean} is corrupted from by adding independent Gaussian noise $N(0,\sigma^2)$

$$y_i := y_{\text{clean}} + \epsilon_i = w \cdot x_i + \epsilon_i \qquad \epsilon_i \sim N(0, \sigma^2)$$

- (x_i, y_i) is revealed as the i^{th} sample

$$(x_1, y_1), \ldots, (x_n, y_n) =: S$$

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Linear Regression: Statistical Modeling View

How can we determine *w*, from Gaussian noise corrupted observations?

$$S = (x_1, y_1), \ldots, (x_n, y_n)$$

Observation:

$$y_i \sim w \cdot x_i + N(0, \sigma^2) = N(w \cdot x_i, \sigma^2)$$

How to estimate parameters of a Gaussian?

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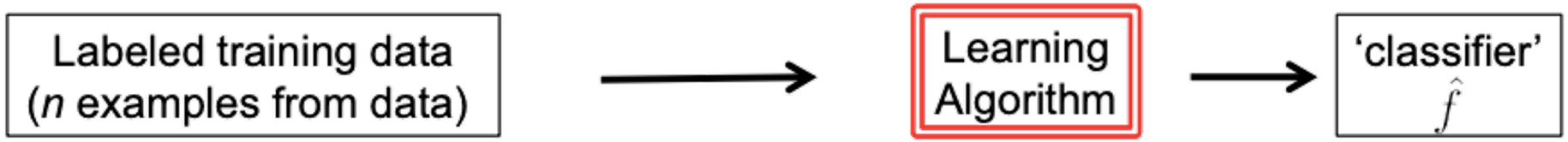
Learning Paradigms

Statistical modeling approach:



$(\vec{x}_1, y_1), (\vec{x}_2, y_2), \ldots (\vec{x}_n, y_n)$

drawn **independently** from
a fixed underlying distribution
(also called the *i.i.d.* assumption)

select $\hat{f}$ from…?
from a pool of ***models*** $\mathcal{F}$
that **maximizes**
label agreement of the
training data

How to select $\hat{f} \in \mathcal{F}$?

- Maximum likelihood (best fits the data)
- Maximum a posteriori (best fits the data but incorporates prior assumptions)
- Optimization of 'loss' criterion (best discriminates the labels)
- …

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Maximum Likelihood Estimation

Given some data $\vec{x}_1, \vec{x}_2, \ldots \vec{x}_n \in \mathcal{X}$ i.i.d. *(Let's forget about the labels for now)*

Say we have a model class $\mathcal{P} = \{p_\theta \mid \theta \in \Theta\}$

ie, each model *p* can be described by a set of parameters θ

find the parameter settings θ that **best fits** the data.

If each model *p*, is a **probability model** then we can find the best fitting probability model via the ***likelihood estimation***!

Likelihood $\mathcal{L}(\theta|X) := P(X|\theta) = P(\vec{x}_1, \ldots, \vec{x}_n|\theta) \overset{\textit{i.i.d.}}{=} \prod_{i=1}^{n} P(\vec{x}_i|\theta) = \prod_{i=1}^{n} p_\theta(\vec{x}_i)$

Interpretation: How **probable** (or how likely) is the data given the model p_θ?

Parameter setting θ that maximizes $\mathcal{L}(\theta|X)$

$$\arg\max_\theta \mathcal{L}(\theta|X) = \arg\max_\theta \prod_{i=1}^{n} p_\theta(\vec{x}_i)$$

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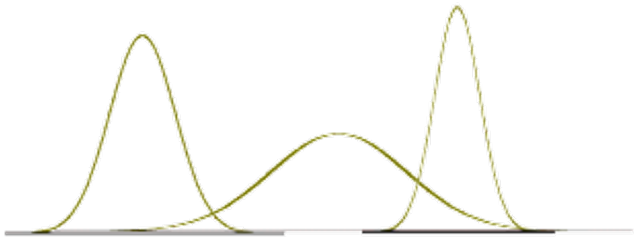
MLE Example

Fitting a statistical probability model to heights of females

Height data (in inches): 60, 62, 53, 58, … $\in \mathbf{R}$

$$x_1, x_2, \ldots x_n \in \mathcal{X}$$

Model class: Gaussian models in **R**



$$p_\theta(x) = p_{\{\mu,\sigma^2\}}(x) := \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

μ = mean parameter

σ^2 = variance parameter > 0

So, what is the MLE for the given data X ?

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MLE Example

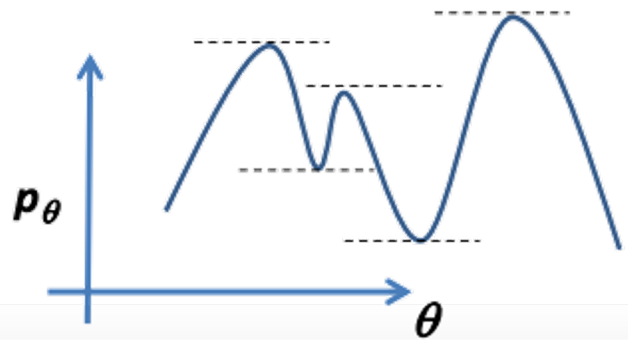
Height data (in inches): $x_1, x_2, \ldots x_n \in \mathcal{X}$ = **R**

Model class: Gaussian models in **R** $p_{\{\mu,\sigma^2\}}(x) := \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2} \right)$

MLE: $\arg\max_{\theta} \mathcal{L}(\theta|X) = \arg\max_{\mu,\sigma^2} \prod_{i=1}^{n} p_{\{\mu,\sigma^2\}}(x_i)$ *Good luck!*

Trick #1: $\arg\max_{\theta} \mathcal{L}(\theta|X) = \arg\max_{\theta} \log \mathcal{L}(\theta|X)$ *"Log" likelihood*

Trick #2: finding max (or other extreme values) of a function is simply analyzing the '**stationary points**' of a function. That is, values at which the **derivative** of the function is zero !



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MLE Example

Let's calculate the best fitting $\theta = \{\mu, \sigma^2\}$

$$\begin{aligned}
\arg\max_{\theta} \mathcal{L}(\theta|X) &= \arg\max_{\theta} \log \mathcal{L}(\theta|X) && \text{"Log" likelihood} \\
&= \arg\max_{\mu,\sigma^2} \log\Big(\prod_{i=1}^{n} p_{\{\mu,\sigma^2\}}(x_i)\Big) && \text{i.i.d.} \\
&= \arg\max_{\mu,\sigma^2} \sum_{i=1}^{n} \log\Big(p_{\{\mu,\sigma^2\}}(x_i)\Big) \\
&= \arg\max_{\mu,\sigma^2} \sum_{i=1}^{n} \Big[\underbrace{-\frac{1}{2}\log(2\pi\sigma^2) - \frac{(x_i-\mu)^2}{2\sigma^2}}_{g_i(\mu,\sigma^2)}\Big]
\end{aligned}$$

Maximizing μ:

$$0 = \nabla_{\mu}\Big(\sum_{i=1}^{n} g_i(\mu,\sigma^2)\Big) \implies \mu_{\mathrm{ML}} = \frac{1}{n}\sum_{i=1}^{n} x_i$$

Maximizing σ^2:

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

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MLE Example

Let's calculate the best fitting $\theta = \{\mu, \sigma^2\}$

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Maximizing μ :

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Maximizing σ^2:

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

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Back to Linear Regression

How can we determine *w*, from Gaussian noise corrupted observations?

$$S = (x_1, y_1), \ldots, (x_n, y_n)$$

Observation:

$$y_i \sim w \cdot x_i + N(0, \sigma^2) = N(w \cdot x_i, \sigma^2)$$

How to estimate parameters of a Gaussian?

Let's try Maximum Likelihood Estimation!

parameter

$$\log \mathcal{L}(w|S) = \sum_{i=1}^{n} \log p(y_i|w)$$

$$\propto \sum_{i=1}^{n} \frac{-(w \cdot x_i - y_i)^2}{2\sigma^2}$$

ignoring terms independent of w

optimizing for w yields the same ols result!

What happens if we model each y_i with indep. noise of different variance?

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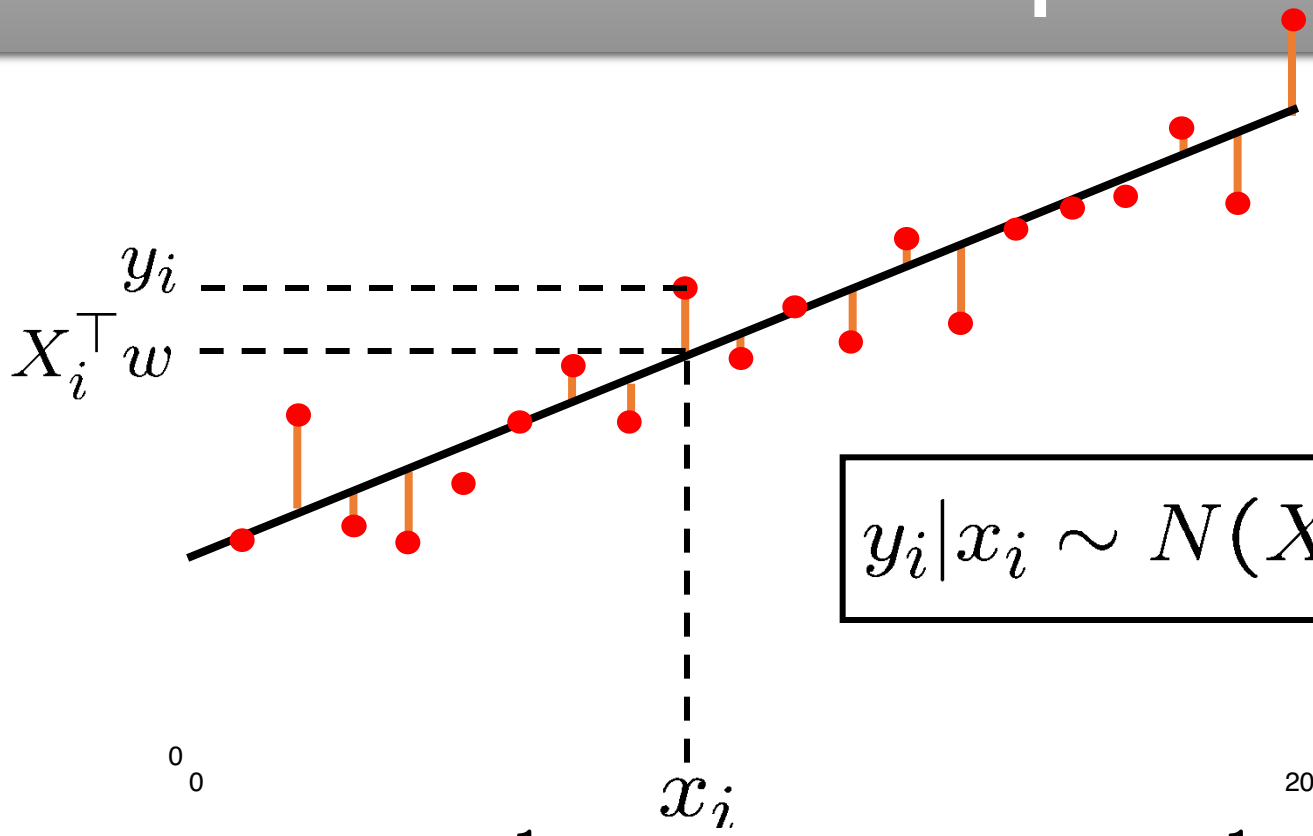
Probabilistic Interpretation



$$y_i | x_i \sim N(X_i^\top w, \sigma^2)$$

Likelihood $$L = \prod_i \exp -\frac{1}{2\sigma^2}(X_i^\top w - y_i)^2 = \exp -\frac{1}{2\sigma^2}\sum_i (X_i^\top w - y_i)^2$$

$$\underset{w}{\text{argmax}}\, L = \underset{w}{\text{argmin}}\, E$$

Regularized Least-Squared Regression

- Complex models (lots of parameters) often prone to overfitting.
- Overfitting can be reduced by imposing a constraint on the overall magnitude of the parameters.
- Two common types of regularization in linear regression:
  - **L_2 regularization (a.k.a. ridge regression):** Find **w** which minimizes:

$$\sum_{j=1}^{N}(y_j - \sum_{i=0}^{d} w_i \cdot x_i)^2 + \lambda \sum_{i=1}^{d} w_i^2$$

    - λ is the regularization parameter: bigger λ imposes more constraint
  - **L_1 regularization (a.k.a. lasso):** Find **w** which minimizes:

$$\sum_{j=1}^{N}(y_j - \sum_{i=0}^{d} w_i \cdot x_i)^2 + \lambda \sum_{i=1}^{d} |w_i|$$

Regularized Least-Squared Regression

- Understanding norms and regularization
  - L_p-norms:

Solving Ridge Regression

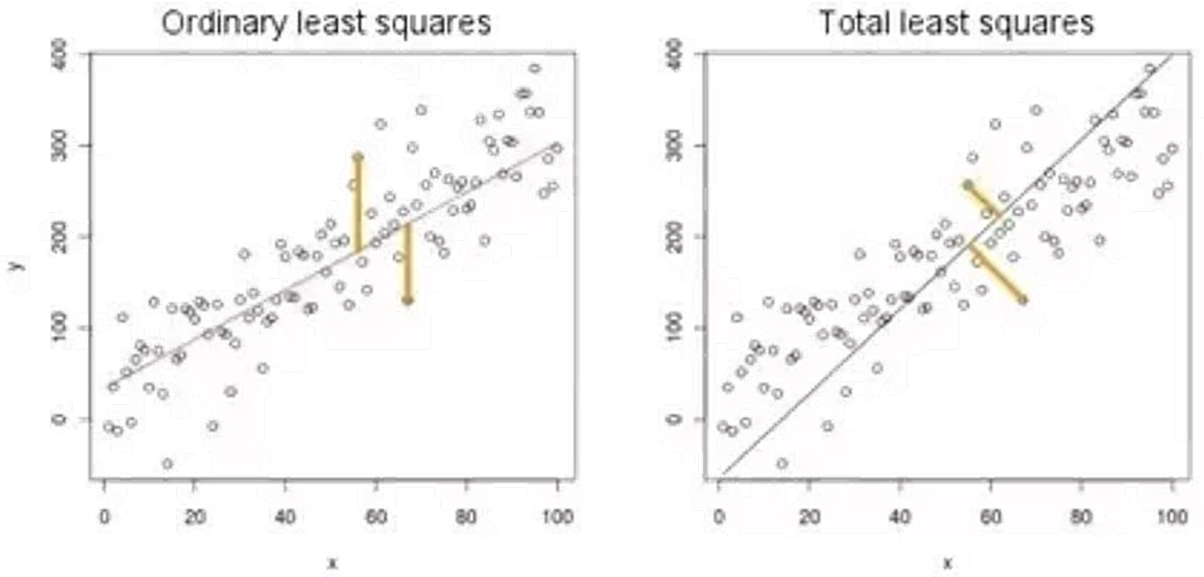
- Minimizing $\lambda \|\mathbf{w}\|^2 + \|\mathbf{y} - \mathbf{X}\mathbf{w}\|^2$ over **w**, we get

$$\left(\mathbf{X}'\mathbf{X} + \lambda \mathbf{I}_n\right)\mathbf{w} = \mathbf{X}'\mathbf{y}$$

- Solution: $\mathbf{w} = \left(\mathbf{X}'\mathbf{X} + \lambda \mathbf{I}\right)^{-1} \mathbf{X}'\mathbf{y}$
- How is this different from the solution for OLS (Ordinary Least-Squares Regression)?
  - Inverse always exists for any $\lambda > 0$.

Total Least Squares and Partial Least Squares

- **Total Least Squares:** Model error in output and input
- **Partial Least Squares:**
  - Seeks to address the correlation between predictor variables in its model
  - Also called "Projection to Latent Structures" (PLS)



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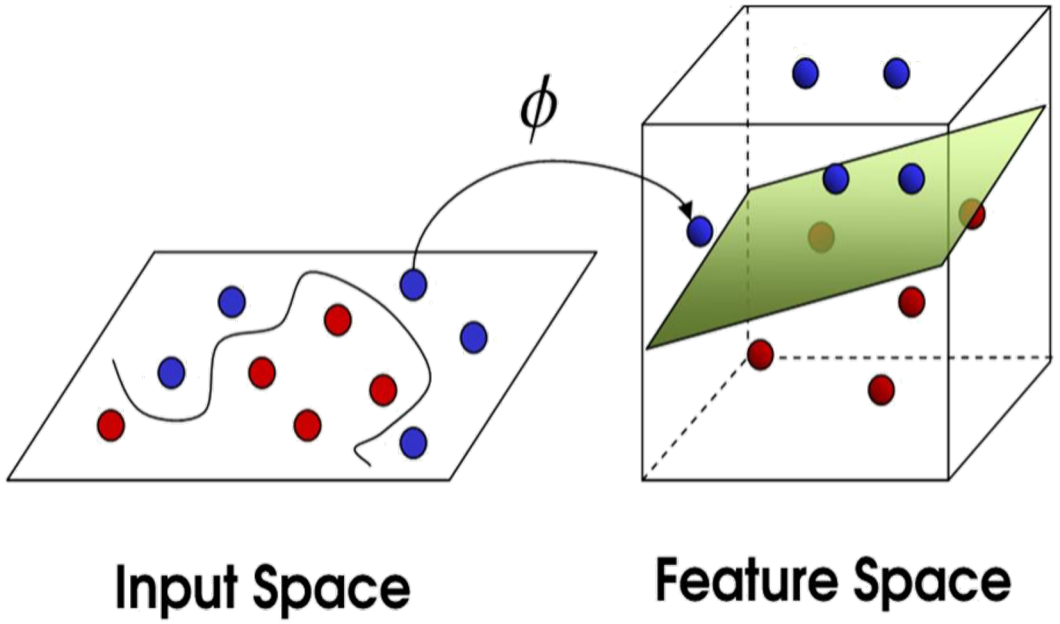
Non-Linear Regression

- Recall: "kernel trick"
- **Key Idea:** Map data to higher dimensional space (feature space) and perform linear regression in embedded space



Non-Linear/Kernel Regression

- Alternative view to ridge regression solution:

$$\mathbf{w} = \left(\mathbf{X}'\mathbf{X} + \lambda \mathbf{I}\right)^{-1} \mathbf{X}'\mathbf{y}$$

Solving is $O(d^3)$

$$\left(\mathbf{X}'\mathbf{X} + \lambda \mathbf{I}\right)\mathbf{w} = \mathbf{X}'\mathbf{y} \Rightarrow \mathbf{w} = \lambda^{-1}\left(\mathbf{X}'\mathbf{y} - \mathbf{X}'\mathbf{X}\mathbf{w}\right)$$

$$\Rightarrow \mathbf{w} = \lambda^{-1}\mathbf{X}'\left(\mathbf{y} - \mathbf{X}\mathbf{w}\right) = \mathbf{X}'\boldsymbol{\alpha}$$

$$\boldsymbol{\alpha} = \lambda^{-1}\left(\mathbf{y} - \mathbf{X}\mathbf{w}\right)$$

$$\Rightarrow \lambda\boldsymbol{\alpha} = \left(\mathbf{y} - \mathbf{X}\mathbf{w}\right) = \left(\mathbf{y} - \mathbf{X}\mathbf{X}'\boldsymbol{\alpha}\right)$$

$$\Rightarrow \mathbf{X}\mathbf{X}'\boldsymbol{\alpha} + \lambda\boldsymbol{\alpha} = \mathbf{y}$$

$$\Rightarrow \boldsymbol{\alpha} = \left(\mathbf{G} + \lambda \mathbf{I}_\ell\right)^{-1}\mathbf{y} \text{ where } \mathbf{G} = \mathbf{X}\mathbf{X}'$$

Do you spot anything interesting?

Solving is $O(n^3)$

Non-Linear/Kernel Regression

- To predict new point:

$$g(\mathbf{x}) = \langle \mathbf{w}, \mathbf{x} \rangle = \left\langle \sum_{i=1}^{d} \alpha_i \mathbf{x}_i, \mathbf{x} \right\rangle = \mathbf{y}' \left(\mathbf{G} + \lambda \mathbf{I} \right)^{-1} \mathbf{z}$$

$$\text{where} \quad \mathbf{z} = \langle \mathbf{x}_i, \mathbf{x} \rangle$$

- Need to only compute G, the Gram Matrix (or the inner products between data points)

$$\mathbf{G} = \mathbf{X}\mathbf{X}' \qquad G_{ij} = \langle \mathbf{x}_i, \mathbf{x}_j \rangle$$

Kernel Ridge Regression

- To predict new point:

$$g(\phi(\mathbf{x})) = \langle \mathbf{w}, \phi(\mathbf{x}) \rangle = \left\langle \sum_{i=1}^{\ell} \alpha_i \phi(\mathbf{x}_i), \phi(\mathbf{x}) \right\rangle = \mathbf{y}' \left(\mathbf{G} + \lambda \mathbf{I} \right)^{-1} \mathbf{z}$$

$$\text{where} \quad \mathbf{z} = \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}) \rangle$$

- Use kernel to compute inner products

$$\mathbf{G} = \phi(\mathbf{X})\phi(\mathbf{X})' \qquad G_{ij} = \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle = K(\mathbf{x}_i, \mathbf{x}_j)$$

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k-NN Regression

- Calculate the mean value of the *k* nearest training examples rather than calculate their most common value

$$f : \Re^d \rightarrow \Re \qquad \hat{f}(x_q) \leftarrow \frac{\sum_{i=1}^{k} f(x_i)}{k}$$

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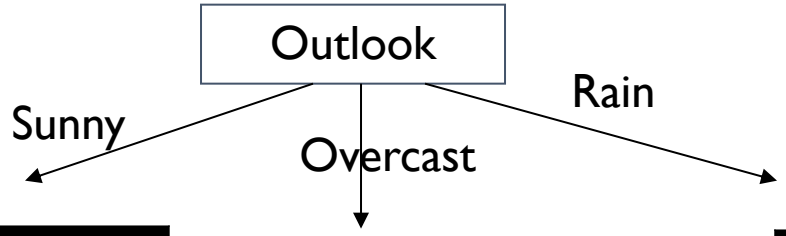
Recall: Decision Trees

- Choose « best » attribute
- Split the learning sample
- Proceed recursively until each object is correctly classified



Day	Outlook	Temp.	Humidity	Wind	Play
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Hot	Normal	Weak	Yes
D11	Sunny	Cool	Normal	Strong	Yes

Day	Outlook	Temp.	Humidity	Wind	Play
D3	Overcast	Hot	High	Weak	Yes
D7	Overcast	Cool	High	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes

Day	Outlook	Temp.	Humidity	Wind	Play
D4	Rain	Mild	Normal	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D10	Rain	Mild	Normal	Strong	Yes
D14	Rain	Mild	High	Strong	No

Recall: Decision Trees

- The "best" split is the split that maximizes the expected reduction of impurity

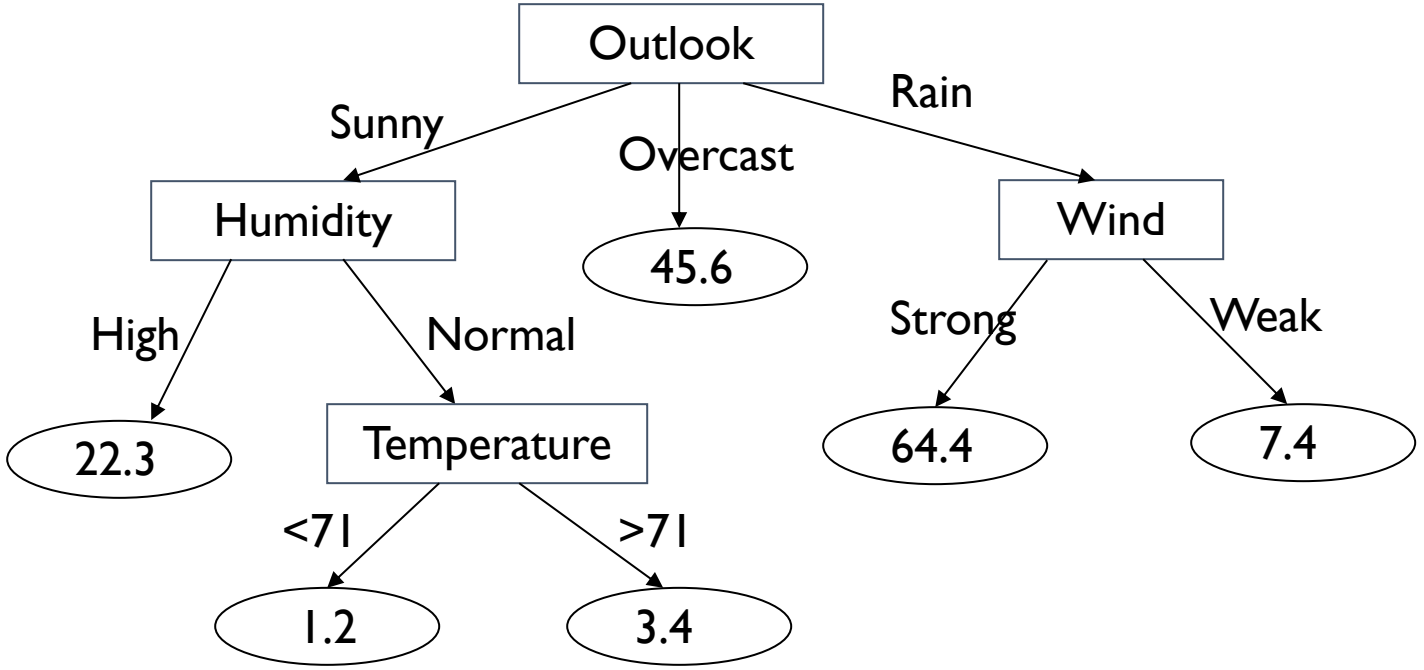
$$\Delta I(LS, A) = I(LS) - \sum_a \frac{|LS_a|}{|LS|} I(LS_a)$$

where LS_a is the subset of records from LS (dataset) such that $A=a$

- Example of impurity measure:
  - *Shannon entropy:* $I(LS) = -\sum_j p_j \log p_j$
  - If two classes, $p_1 = 1 - p_2$
  - The reduction of entropy is called the information gain

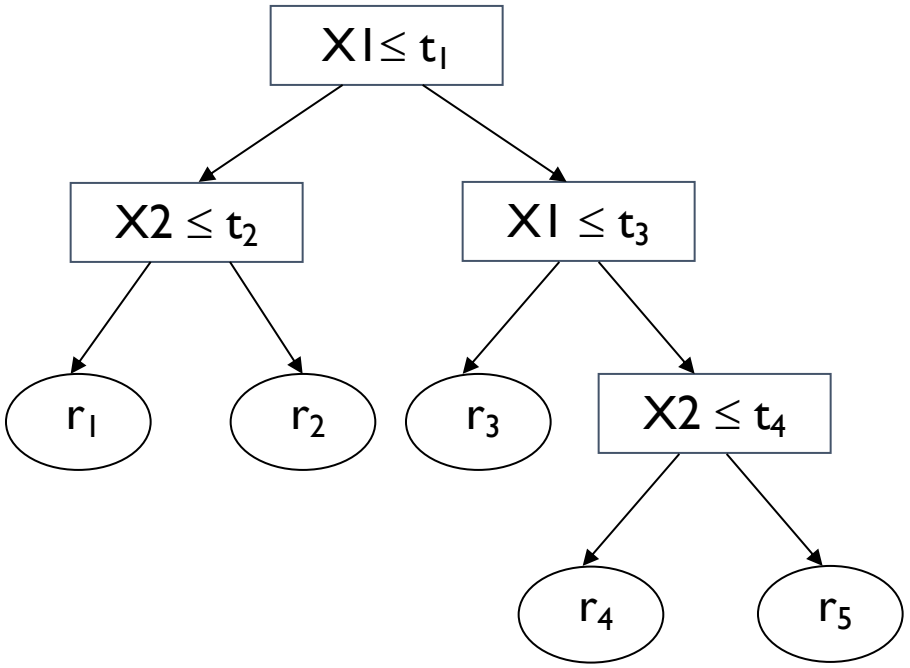
Regression Trees

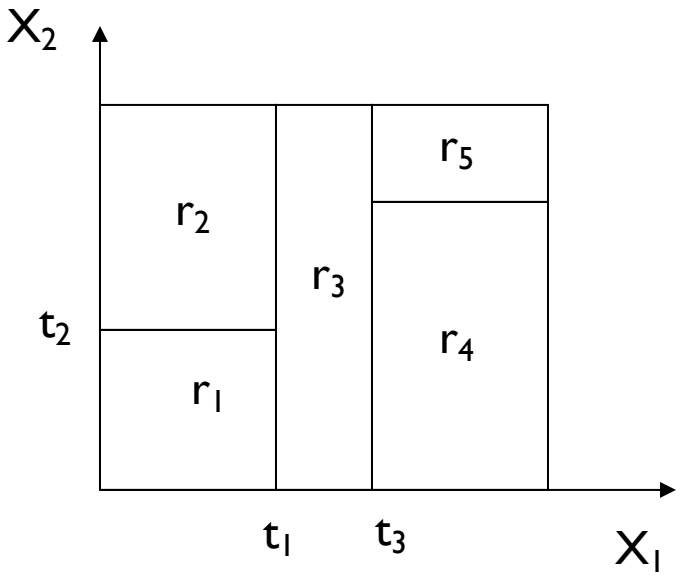
- Tree for regression: exactly the same model but with a number in each leaf instead of a class



Regression Trees

- A regression tree is a piecewise constant function of the input attributes





Growing Regression Trees

- To minimize the square error on the learning sample, the prediction at a leaf is the average output of the learning cases reaching that leaf
- Impurity of a sample is defined by the variance of the output in that sample:

$$I(LS)=var_{y|LS}\{y\}=E_{y|LS}\{(y-E_{y|LS}\{y\})^2\}$$

- The best split is the one that reduces the most variance:

$$\Delta I(LS,A) = \text{var}_{y|LS}\{y\} - \sum_a \frac{|LS_a|}{|LS|} \text{var}_{y|LS_a}\{y\}$$

Regression Tree Pruning

- Exactly the same algorithms apply: pre-pruning and post-pruning.
- In practice, pruning is more important in regression because full trees are much more complex
  - Each data instance can have a different output value and hence the full tree has as many leaves as there are training instances

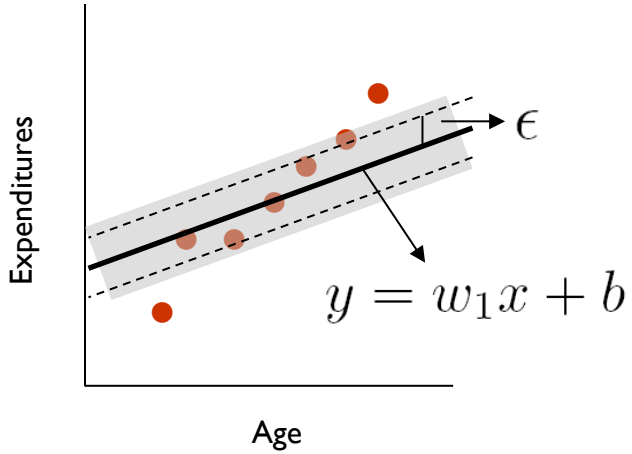
Regression Methods

- Linear Least-Squares Regression
  - Partial Least-Squares
  - Total Least-Squares
  - Ridge Regression, LASSO
- Kernel Regression
- k-NN Regression
- Regression Trees
- Support Vector Regression
- Logistic Regression

Support Vector Regression

- Given training data $\{x_i, y_i\}_{i=1}^{n}$
- Find: w_1 and b ,

  such that $y = w_1 x + b$ optimally describes the data:



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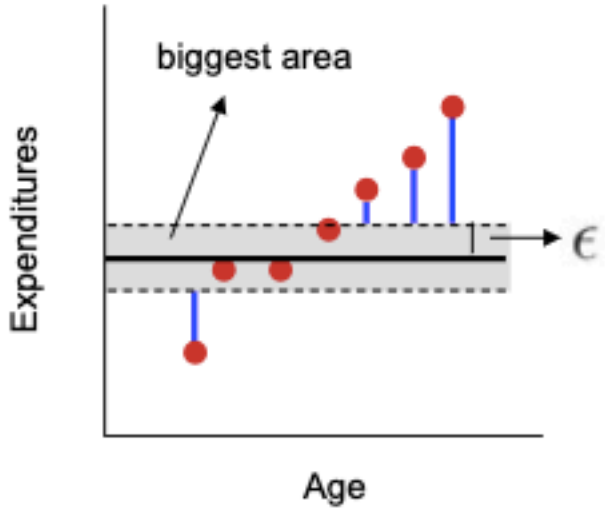
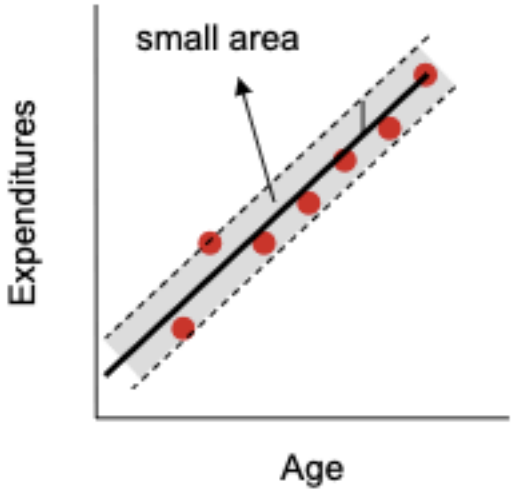
Support Vector Regression



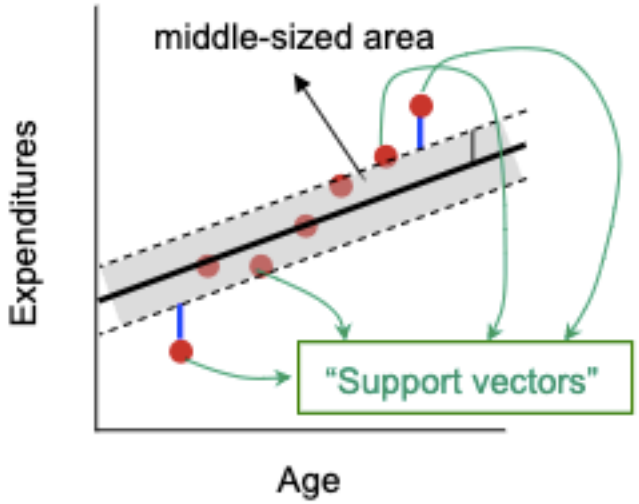
"Lazy case"

(underfitting)



"Suspiciously smart case"

(overfitting)



"Compromise case", SVR

(good generalizability)

- **The thinner the "tube", the more complex the model**

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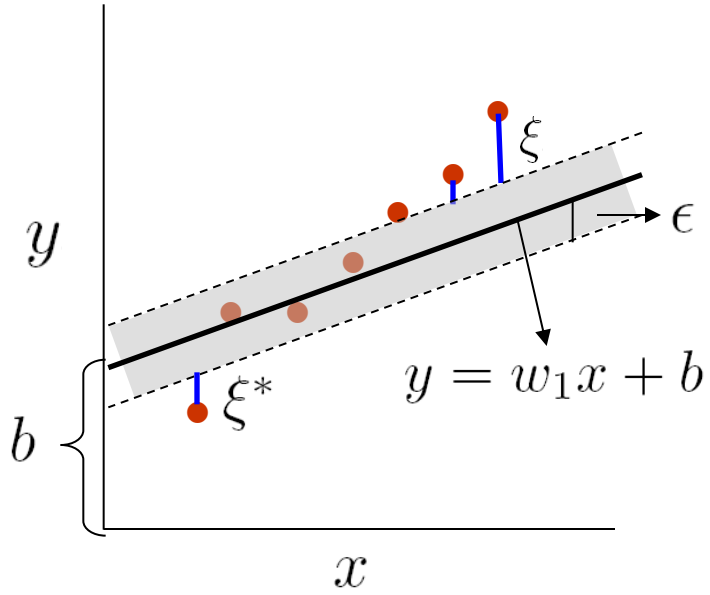
Support Vector Regression



$| w_1 |$ vs. $\sum_i (\xi_i + \xi_i^*)$

Complexity — Sum of errors

$$\min_{w_1, b, \xi_i, \xi_i^*} \frac{1}{2} w_1^2 + C \sum_i (\xi_i + \xi_i^*)$$

Case I: $w_1 \downarrow$ → "tube" $\uparrow$ → complexity $\downarrow$ → $\sum_i (\xi_i + \xi_i^*) \uparrow$

Case II: $w_1 \uparrow$ → "tube" $\downarrow$ → complexity $\uparrow$ → $\sum_i (\xi_i + \xi_i^*) \downarrow$

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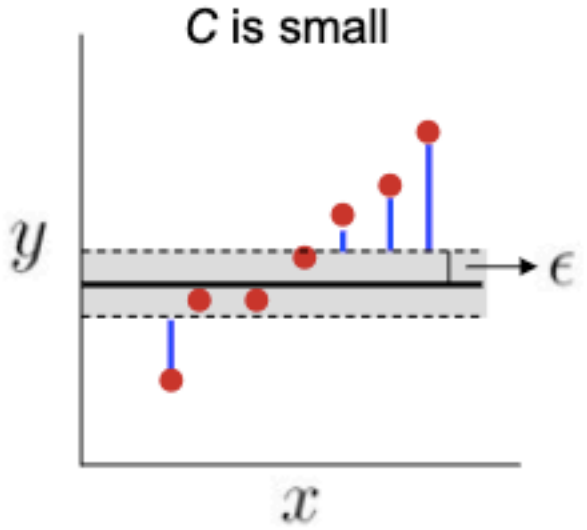
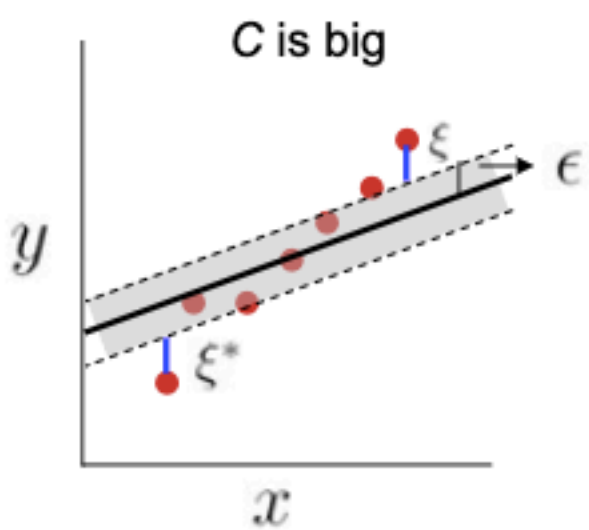
Support Vector Regression



- The role of C



Case I: $w_1 \downarrow$ → "tube" $\uparrow$ → complexity $\downarrow$ → $\sum_i(\xi_i + \xi_i^*) \uparrow$

Case II: $w_1 \uparrow$ → "tube" $\downarrow$ → complexity $\uparrow$ → $\sum_i(\xi_i + \xi_i^*) \downarrow$

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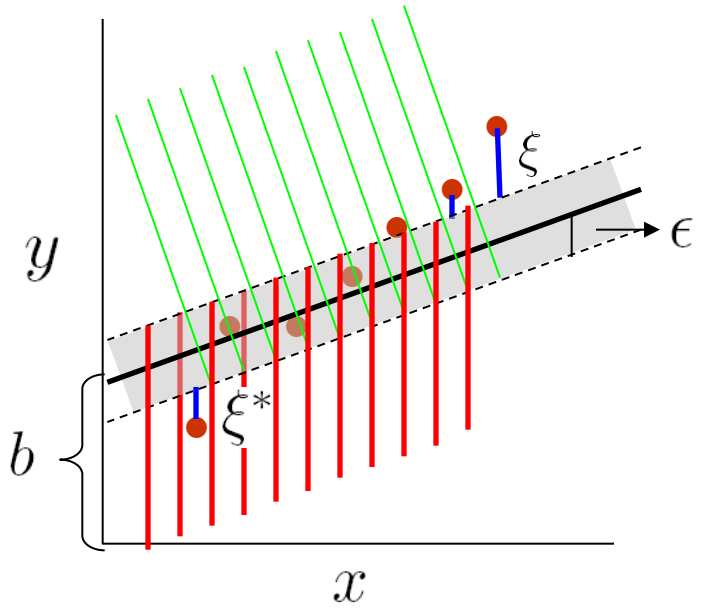
Support Vector Regression



$$y = w_1 x + b$$

$$\min_{w_1, b, \xi_i, \xi_i^*} \quad \frac{1}{2} w_1^2 + C \sum_i (\xi_i + \xi_i^*)$$

Subject to:

$$y_i - (w_1 x_{i1}) - b \leq \epsilon + \xi_i$$

$$(w_1 x_{i1}) + b - y_i \leq \epsilon + \xi_i^*$$

$$\xi_i, \xi_i^* \geq 0 \quad i = 1, 2, \ldots, n$$

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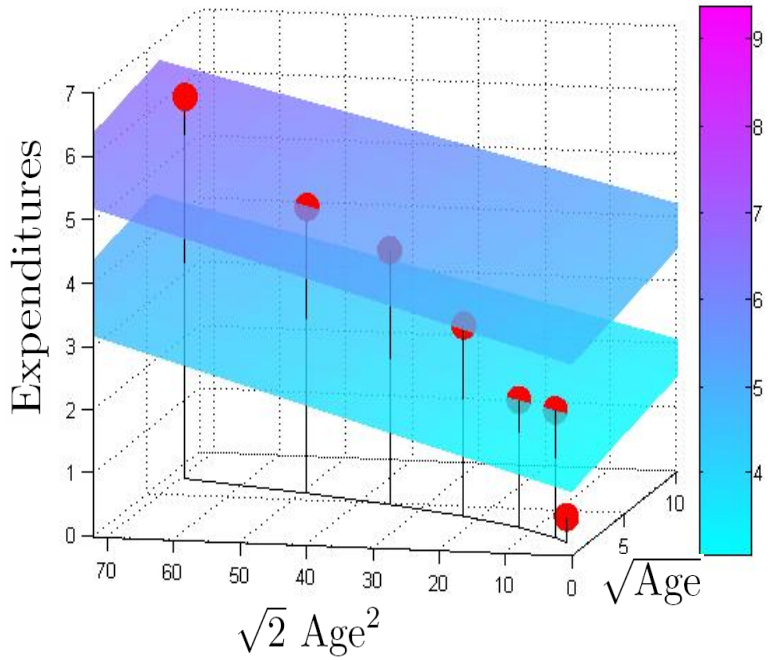
Non-linear (Kernel) SVR



$$y = \mathbf{w}'\Phi(x) + b$$

$$\min_{w_1, b, \xi_i, \xi_i^*} \frac{w_1^2 + w_2^2}{2} + C \sum_i (\xi_i + \xi_i^*)$$

Subject to:

$$y_i - (\mathbf{w}'\phi(x_{i1})) - b \leq \epsilon + \xi_i$$
$$(\mathbf{w}'\phi(x_{i1})) + b - y_i \leq \epsilon + \xi_i^*$$
$$\xi_i, \xi_i^* \geq 0 \qquad i = 1, 2, \ldots, n$$

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SVR: Derivation

$$\min_{\mathbf{w},b,\xi_i,\xi_i^*} \quad \frac{1}{2} \parallel \mathbf{w} \parallel^2 + C \sum_i (\xi_i + \xi_i^*)$$

Subject to:

$$y_i - (\mathbf{w}'\phi(\mathbf{x}_i)) - b \leq \epsilon + \xi_i$$
$$(\mathbf{w}'\phi(\mathbf{x}_i))) + b - y_i \leq \epsilon + \xi_i^*$$
$$\xi_i, \xi_i^* \geq 0 \qquad i = 1, 2, \ldots, n$$

$$L := \frac{1}{2} \parallel \mathbf{w} \parallel^2 + C \sum_i (\xi_i + \xi_i^*) - \sum_i (\eta_i \xi_i + \eta_i^* \xi_i^*)$$
$$- \sum_i \alpha_i (\epsilon + \xi_i - y_i + \mathbf{w}'\phi(\mathbf{x}_i) + b) - \sum_i \alpha_i^* (\epsilon + \xi_i^* + y_i - \mathbf{w}'\phi(\mathbf{x}_i)) - b)$$

min with respect to $\mathbf{w}, b, \xi_i, \xi_i^*$

max with respect to $\alpha_i, \alpha_i^*, \eta_i, \eta_i^*$

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SVR: Summary

- Strengths of SVR:
  - No local minima
  - Scales relatively well to high-dimensional data
  - Trade-off between classifier complexity and error can be controlled explicitly via *C* and *epsilon*
  - Overfitting is avoided (for any fixed *C* and *epsilon*)
  - The "curse of dimensionality" is avoided through kernel functions
- Weaknesses of SVR:
  - What is the best trade-off parameter *C* and best *epsilon*?
  - What is a *good* transformation of the original space?

Regression Methods

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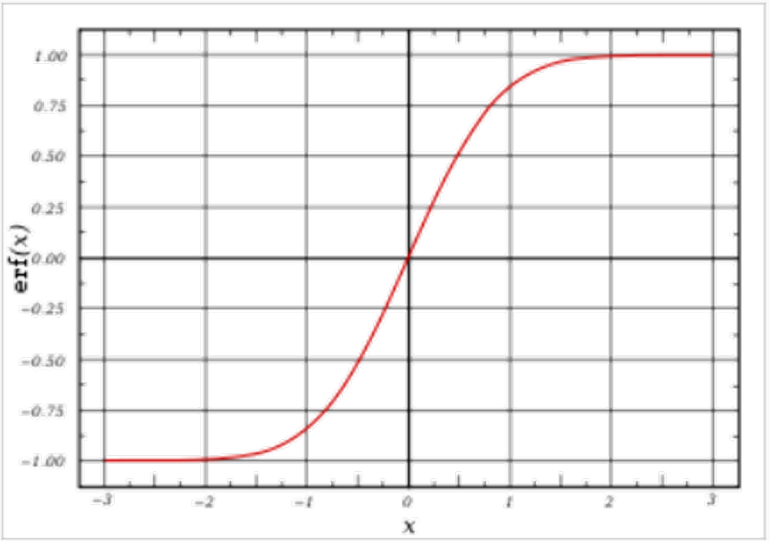
  - Partial Least-Squares
  - Total Least-Squares
  - Ridge Regression, LASSO
- Kernel Regression
- k-NN Regression
- Regression Trees
- Support Vector Regression
- Logistic Regression

Logistic Regression

- To predict an outcome variable that is categorical from one or more categorical or continuous predictor variables.
- Used because having a categorical outcome variable violates the assumption of linearity in normal regression.

- Let X be the data instance, and Y be the class label: Learn P(Y|X) directly
  - Let W = ($W_1, W_2, \ldots W_n$), X=($X_1, X_2, \ldots, X_n$), **W.X** is the dot product
  - Sigmoid function: $$P(Y=1|\mathbf{X}) = \frac{1}{1+e^{-\mathbf{wx}}}$$



Logistic Regression

- Generative or Discriminative?

Logistic Regression

- Generative classifier, e.g., Naïve Bayes:
  - Assume some functional form for **P(X|Y), P(Y)**
  - Estimate parameters of P(X|Y), P(Y) directly from training data
  - Use Bayes rule to calculate P(Y|X=x)
  - This is 'generative' model
    - Indirect computation of P(Y|X) through Bayes rule
    - But, can generate a sample of the data, $P(X) = \sum_y P(y)P(X \mid y)$
- Discriminative classifier, e.g., Logistic Regression:
  - Assume some functional form for **P(Y|X)**
  - Estimate parameters of P(Y|X) directly from training data
  - This is the 'discriminative' model
    - Directly learn P(Y|X)

Logistic Regression

- In logistic regression, we learn the conditional distribution P(y|x)
- Let $p_y(x;w)$ be our estimate of P(y|x), where w is a vector of adjustable parameters.
- Assume there are two classes, y = 0 and y = 1 and

$$p_1(\mathbf{x};\mathbf{w}) = \frac{1}{1+e^{-\mathbf{wx}}} \qquad p_0(\mathbf{x};\mathbf{w}) = 1 - \frac{1}{1+e^{-\mathbf{wx}}}$$

- This is equivalent to $\log \frac{p_1(\mathbf{x};\mathbf{w})}{p_0(\mathbf{x};\mathbf{w})} = \mathbf{wx}$

- That is, the log odds of class 1 is a linear function of x
- Q: How to find **W**?

Logistic Regression

- Conditional data likelihood - Probability of observed Y values in the training data, conditioned on corresponding X values.
- We choose parameters w that satisfy

$$\mathbf{w} = \arg\max_{\mathbf{w}} \prod_{l} P(y^l \mid \mathbf{x}^l, \mathbf{w})$$

- where
  - $\mathbf{w} = \langle w_0, w_1, \ldots, w_n \rangle$ is the vector of parameters to be estimated,
  - y^l denotes the observed value of Y in the *l* th training example, and
  - $\mathbf{x}^l$ denotes the observed value of **X** in the *l* th training example

Logistic Regression

- Equivalently, we can work with log of conditional likelihood:

$$\mathbf{w} = \arg\max_{\mathbf{w}} \sum_{l} \ln P(y^l \mid \mathbf{x}^l, \mathbf{w})$$

- Conditional data log likelihood, l(W), can be written as

$$l(\mathbf{w}) = \sum_{l} y^l \ln P(y^l = 1 \mid \mathbf{x}^l, \mathbf{w}) + (1 - y^l) \ln P(y^l = 0 \mid \mathbf{x}^l, \mathbf{w})$$

- Note here that Y can take only values 0 or 1, so only one of the two terms in the expression will be non-zero for any given y^l

Logistic Regression: Training

- We need to estimate:

$$\mathbf{w} = \arg\max_{\mathbf{w}} \sum_{l} \ln P(y^l \mid \mathbf{x}^l, \mathbf{w})$$

- Equivalently, we can minimize negative log likelihood
- This is convex – so, unique global minimum
- No closed-form solution though. Iterative method required.

Logistic Regression: Training

- Use gradient ascent (descent) for the maximization (min) problem
- The i th component of the vector gradient has the form

$$\frac{\partial}{\partial w_i} l(\mathbf{w}) = \sum_l x_i^l (y^l - \hat{P}(y^l = 1 \mid \mathbf{x}^l, \mathbf{w}))$$

Logistic Regression prediction

- Beginning with initial weights, we repeatedly update the weights in the direction of the gradient, changing the i th weight according to

$$w_i \leftarrow w_i + \eta \sum_l x_i^l (y^l - \hat{P}(y^l = 1 \mid \mathbf{x}^l, \mathbf{w}))$$

Regularization in Logistic Regression

- Overfitting can arise especially when data has very high dimensions and is sparse.
- One approach -> modified "penalized log likelihood function," which penalizes large values of **w**, as before.

$$\mathbf{w} = \arg\max_{\mathbf{w}} \sum_{l} \ln P(y^l \mid \mathbf{x}^l, \mathbf{w}) - \frac{\lambda}{2} \| \mathbf{w} \|^2$$

- Derivative then becomes:

$$\frac{\partial}{\partial w_i} l(\mathbf{w}) = \sum_{l} x_i^l (y^l - \hat{P}(y^l = 1 \mid \mathbf{x}^l, \mathbf{w})) - \lambda w_i$$

Logistic Regression: Summary

- In general, NB and LR make different assumptions
  - NB: Features independent given class -> assumption on P(X|Y)
  - LR: Functional form of P(Y|X), no assumption on P(X|Y)
- LR is a linear classifier
  - decision rule is a hyperplane
- LR optimized by conditional likelihood
  - no closed-form solution
  - Concave (convex) -> global optimum with gradient ascent (descent)
- Extending logistic regression to multiple classes?
  - Use softmax for each class k!

$$p(y = k|x) = \frac{\exp(\theta_k^\top x)}{\sum_{i=1}^{K} \exp(\theta_i^\top x)}$$

Other Regression Methods

- Bayesian Regression
- Generalized Regression Neural Network

Readings

- PRML Bishop
  - Sec 3.1, Sec 4.3, Sec 7.1
- "Introduction to Machine Learning" by Ethem Alpaydin
  - Sec 4.6, 5.8, Chap 10, Chap 13
- Other resources
  - A nice tutorial on SVR: https://alex.smola.org/papers/2004/SmoSch04.pdf