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Regularised Least Squares

- **Why?** ■ An otherwise nice model with nice properties, but gives infinite/trivial solutions ■
- To control overfitting ■
- **Start:** ■ $E_D(\mathbf{w}) \triangleq \sum_{i=1}^N \{t_i - \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_i)\}^2$ (data fidelity) ■
- To minimise $E_D(\mathbf{w}) + \lambda E_w(\mathbf{w})$ ■ Fidelity, weights ■
param $\lambda : E_w(\mathbf{w}) = 0$. ■ $E_w(\mathbf{w}) = \frac{1}{2} \mathbf{w}^T \mathbf{w} = \frac{1}{2} \sum_{j=0}^{M-1} w_j^2$ ■
- **Advantage:** ■ Quadratic in \mathbf{w} : ■ closed-form solution ■
- (ML): ■ 'weight decay': ■ weights $\downarrow 0$ unless supported by the data. ■ (Stat): ■ 'param shrinkage' ■
- $E \triangleq \sum_{i=1}^N \{t_i - \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_i)\}^2 + \lambda \frac{1}{2} \mathbf{w}^T \mathbf{w}$. ■ $\frac{\partial E}{\partial \mathbf{w}} = 0$ ■ \implies
■ $\frac{\partial}{\partial \mathbf{w}} \left[\sum_{i=1}^N \{t_i - \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_i)\}^2 + \lambda \frac{1}{2} \mathbf{w}^T \mathbf{w} \right] = 0 \implies$ ■
■ $\sum_{i=1}^N t_i \boldsymbol{\phi}^T(\mathbf{x}_i) = \sum_{i=1}^N \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_i) \boldsymbol{\phi}^T(\mathbf{x}_i) + \lambda \mathbf{w}^T \implies$ ■



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- $\sum_{i=1}^N t_i \phi^T(\mathbf{x}_i) = \mathbf{w}^T (\sum_{i=1}^N \phi(\mathbf{x}_i) \phi^T(\mathbf{x}_i) + \lambda \mathbf{I}) \Rightarrow$

$$\begin{bmatrix} t_1 \\ \vdots \\ t_N \end{bmatrix}^T = \mathbf{w}^T \left(\begin{bmatrix} \phi(\mathbf{x}_1) \\ \vdots \\ \phi(\mathbf{x}_N) \end{bmatrix} \begin{bmatrix} \phi(\mathbf{x}_1)^T \\ \vdots \\ \phi(\mathbf{x}_N)^T \end{bmatrix} + \lambda \mathbf{I} \right) \Rightarrow$$

$$\mathbf{t}^T \Phi = (\Phi^T \Phi + \lambda \mathbf{I})^T \mathbf{w} = (\Phi^T \Phi + \lambda \mathbf{I}) \mathbf{w} \Rightarrow$$

- $\mathbf{w} = (\Phi^T \Phi + \lambda \mathbf{I})^{-1} \Phi^T \mathbf{t}$

- Note about the $\|\mathbf{w}^T \mathbf{w}\|$: May actually be implemented numerically as $\|\mathbf{w}^T \mathbf{w}\| - c$, small c



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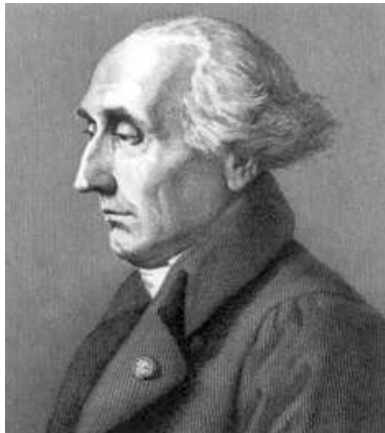
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Intertwined Histories



J.-L. Lagrange
[1736-1813]

https://upload.wikimedia.org/wikipedia/commons/1/19/Lagrange_portrait.jpg



A. Lavoisier
[1743-1794]

<https://upload.wikimedia.org/wikipedia/commons/4/44/Lavoisier-statue.jpg>



J.-B. J. Fourier
[1768-1830]

<https://upload.wikimedia.org/wikipedia/commons/a/aa/Fourier2.jpg>

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Classification

- $\mathbf{x} \rightarrow [\text{Classifier}] \rightarrow \mathcal{C}_j$
- Three approaches to Classification:
 1. Simplest: Discriminant Functions:
Functions which directly assign a class to \mathbf{x} .
Linear Discriminant: the discriminant fns are lines/linear/hyperplanes
 2. Model them directly: e.g., Mixture of Gaussians. Represent as parametric models, optimise params using a training set
 3. Toughest: Generative Approach: Find $P(\mathcal{C}_j|\mathbf{x})$
Find $P(\mathcal{C}_j|\mathbf{x})$ using the Bayes' Theorem:
 $P(\mathcal{C}_j|\mathbf{x}) = P(\mathbf{x}|\mathcal{C}_j)P(\mathcal{C}_j)/P(\mathbf{x})$. Models for:
 $P(\mathbf{x}|\mathcal{C}_j)$: class cond densities; $P(\mathcal{C}_j)$: priors



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Men of God...



Thomas Bayes
[1701-1761]

https://upload.wikimedia.org/wikipedia/commons/d/d4/Thomas_Bayes.gif



G. J. Mendel
[1882-1884]

https://upload.wikimedia.org/wikipedia/commons/3/3d/Gregor_Mendel_oval.jpg



M. Mitra
[1968-]

http://iseeindia.com/wordpress/wp-content/uploads/2011/11/Ramkrishna_Miss11736-290x290.jpg

Mahan Maharaj/Swami Vidyanathananda
2011 Shanti Swarup Bhatnagar Award in Math Sciences
Infosys Prize 2015 for Mathematical Sciences

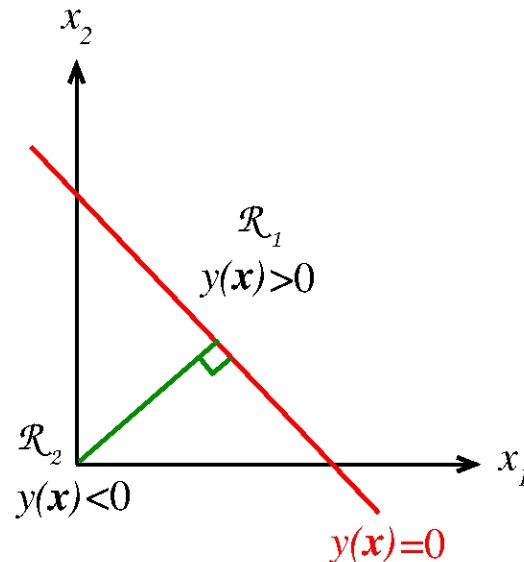
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Useful Generalisations of Linearity

- Linearity: Written equivalently in two ways:
 $y(\mathbf{x}, \mathbf{w}) = \mathbf{w}^T \mathbf{x}$, for $(D+1) = M - \text{dim data}$, $x_0 = 1$, or
 $y(\mathbf{x}, \mathbf{w}) = \mathbf{w}^T \mathbf{x} + w_0$, for $D = (M-1) - \text{dim data}$
- $y(\mathbf{x}, \mathbf{w}) = w_0 x_0 + \dots w_{M-1} x_{M-1} = \sum_{j=0}^{M-1} w_j x_j$
- Model useful for Regression: linear comb of basis fns (lin/non-lin) $y(\mathbf{x}, \mathbf{w}) = \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x})$
- Generalising lin to scalar basis functions $\phi_j(\mathbf{x})$:
 $y(\mathbf{x}, \mathbf{w}) = \sum_{j=0}^{M-1} w_j \phi_j(\mathbf{x}) = w_0 \phi_0(\mathbf{x}) + \dots w_{M-1} \phi_{M-1}(\mathbf{x})$
- Model useful for Classification: fns (lin/non-lin) of the linear $\mathbf{w}^T \mathbf{x}$ (or $\mathbf{w}^T \boldsymbol{\phi}(\mathbf{x})$) $y(\mathbf{x}, \mathbf{w}) = f(\mathbf{w}^T \mathbf{x})$
- Examples: Linear Regression, Neural Networks

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Discriminant Functions: 2 Classes



- $y(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + w_0$
- 2-D implicit form of eqn of a line is $ax + by + c = 0$. Here, $y(\mathbf{x}, \mathbf{w}) = w_2x_2 + w_1x_1 + w_0 = 0$
- $y(\mathbf{x}) = 0$: 1-D h'plane in 2-D
- Relative location of $\mathcal{R}_1, \mathcal{R}_2$ is immaterial: which is above/below/to the left/to the right
- Physical Significance of w_0 : measure of the dist from the origin Why? For $ax + by + c = 0$, perp distance of (x_1, y_1) from the line is $\frac{|ax_1 + by_1 + c|}{\sqrt{a^2 + b^2}}$
Perp dist of $y(\mathbf{x}) = 0$ from the origin = $\frac{|w_2(0) + w_1(0) + w_0|}{\sqrt{w_2^2 + w_1^2}} = \frac{|w_0|}{\|\mathbf{w}\|}$, $\|\mathbf{w}\|^2 = \mathbf{w}^T \mathbf{w} = \sum w_j^2$

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Some more Physical Significance

- For two points \mathbf{x}_A and \mathbf{x}_B on the line $y(\mathbf{x}) = 0$:

$$y(\mathbf{x}_A) = 0 \implies \mathbf{w}^T \mathbf{x}_A + w_0 = 0$$

$$y(\mathbf{x}_B) = 0 \implies \mathbf{w}^T \mathbf{x}_B + w_0 = 0$$

$$\implies \mathbf{w}^T (\mathbf{x}_A - \mathbf{x}_B) = 0 \implies \mathbf{w} \perp \text{line } y(\mathbf{x}) = 0$$

- Phy Significance of perp dist of a point from a line

$$\mathbf{x} = \mathbf{x}_\perp + r \hat{\mathbf{w}} = \mathbf{x}_\perp + r \frac{\mathbf{w}}{\|\mathbf{w}\|}$$

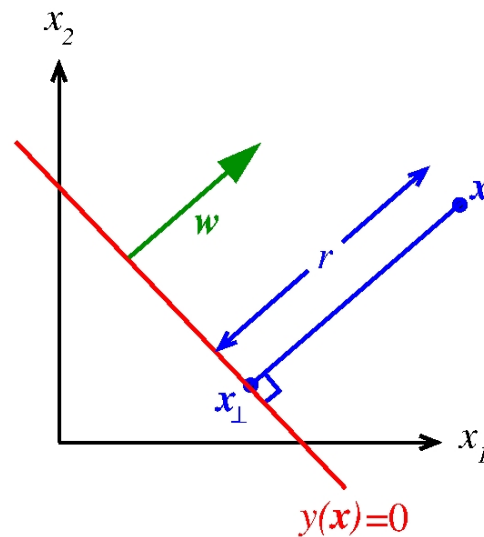
- Pre-multiply by \mathbf{w}^T & add w_0 :

$$\mathbf{w}^T \mathbf{x} + w_0 = \mathbf{w}^T (\mathbf{x}_\perp + r \frac{\mathbf{w}}{\|\mathbf{w}\|}) + w_0$$

$$\implies y(\mathbf{x}) = (\mathbf{w}^T \mathbf{x}_\perp + w_0) + r \frac{\|\mathbf{w}\|^2}{\|\mathbf{w}\|}$$

$$\implies r = \frac{y(\mathbf{x})}{\|\mathbf{w}\|}$$

- Consistent with perp distance of (x_1, y_1) from line: $\frac{ax_1 + by_1 + c}{\sqrt{a^2 + b^2}}$

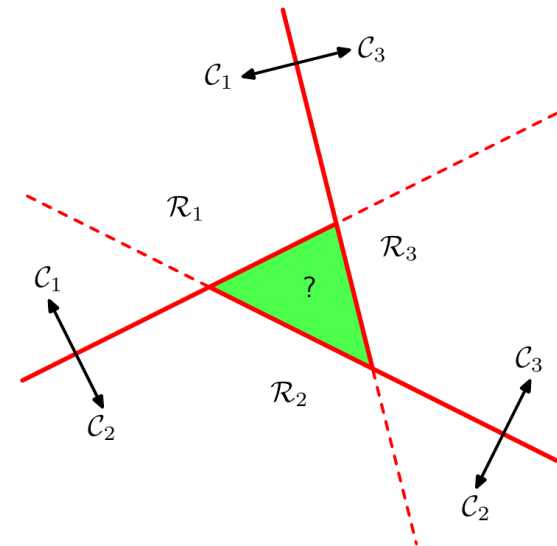
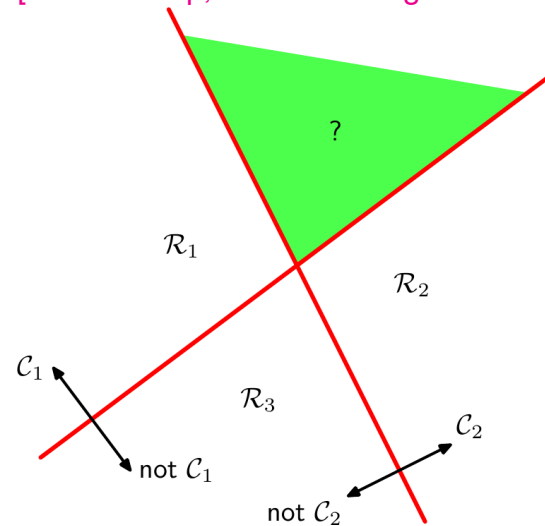


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Discriminant Functions: K Classes

- Building a K – Classifier from 2-class ones

[C. M. Bishop, Pattern Recognition and Machine Learning. Springer, 2006. Fig. 4.2, p. 183]



- One-versus-Rest

- $K - 1$ classifiers, each of which solves the 2-class \mathcal{C}_j vs. not \mathcal{C}_j

- One-versus-One

- $K C_2$ 2-class classifiers
- Ambiguity here also!

- e.g., Tree-SVM? Explicitly define the hierarchy!