Content

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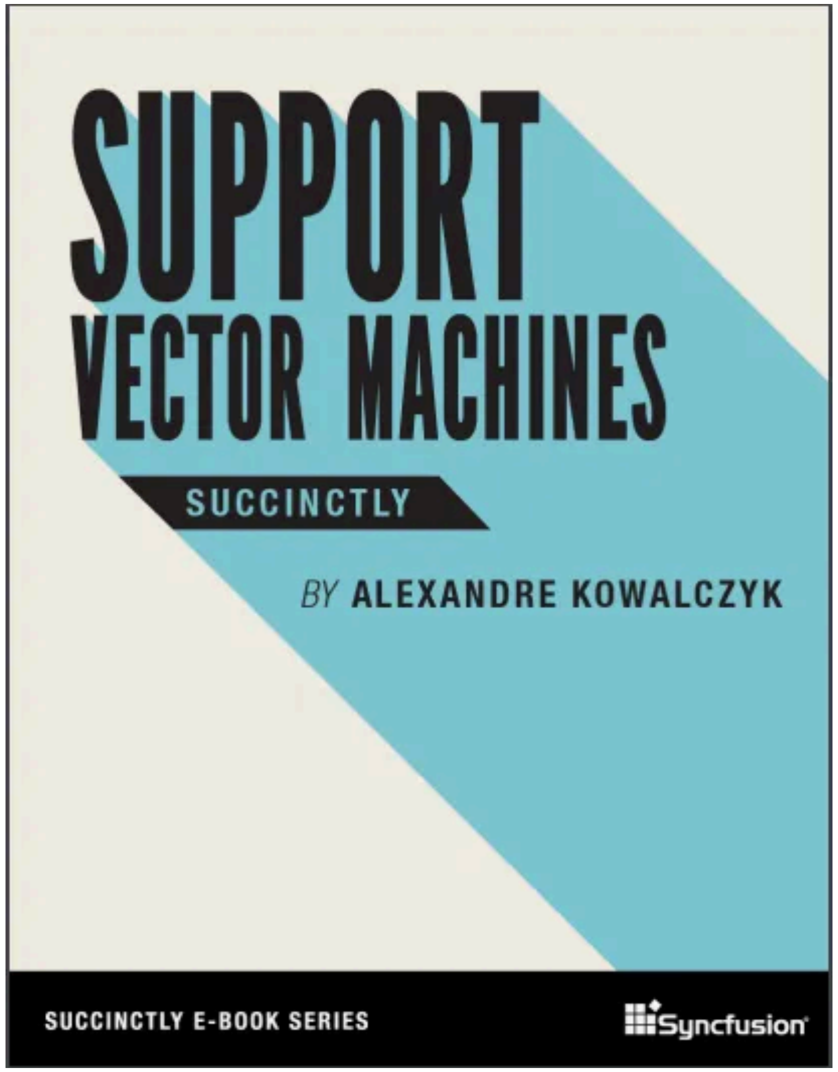
3. Neural Networks
   - 3.1 Biological neural networks
   - 3.2 Mathematical representation
   - 3.3 Factoring biological ingredient
   - 3.4 Feed-forward neural networks
   - 3.5 Learning algorithm
   - 3.6 Universal Approximation Theorem

Support Vector Machine

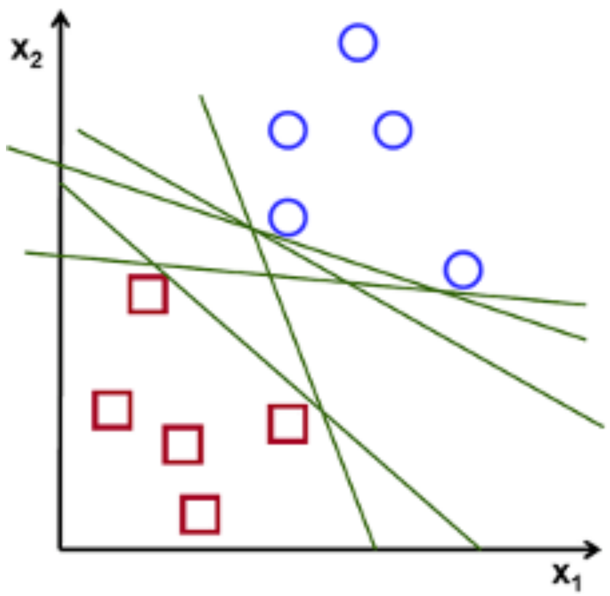
Good references by Alexandre Kowalczyk

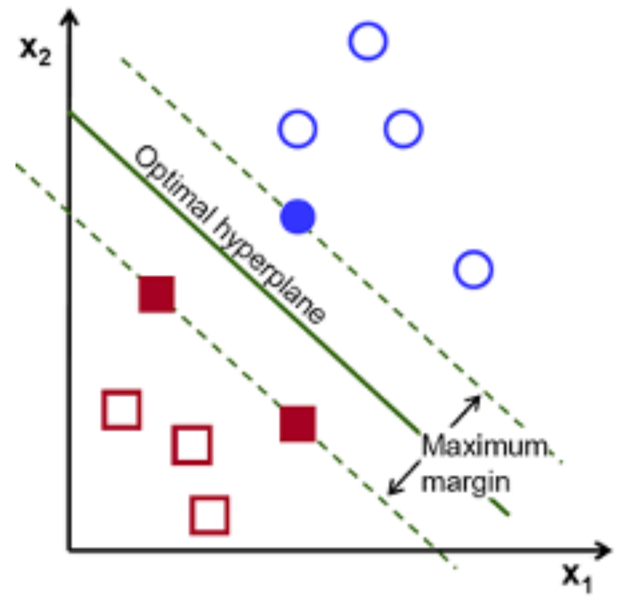
https://www.svm-tutorial.com/

https://www.syncfusion.com/ebooks/support_vector_machines_succinctly



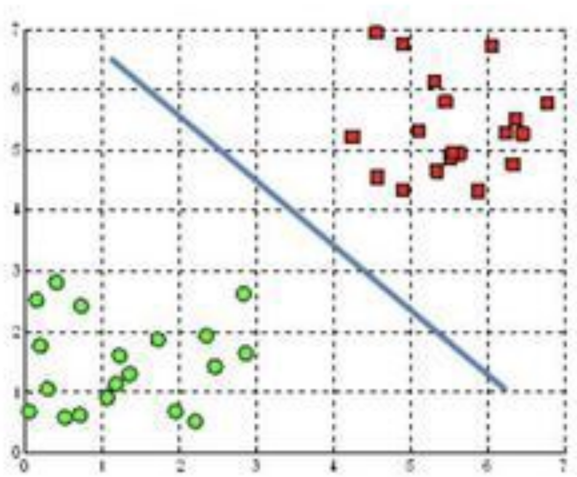
Support Vector Machine

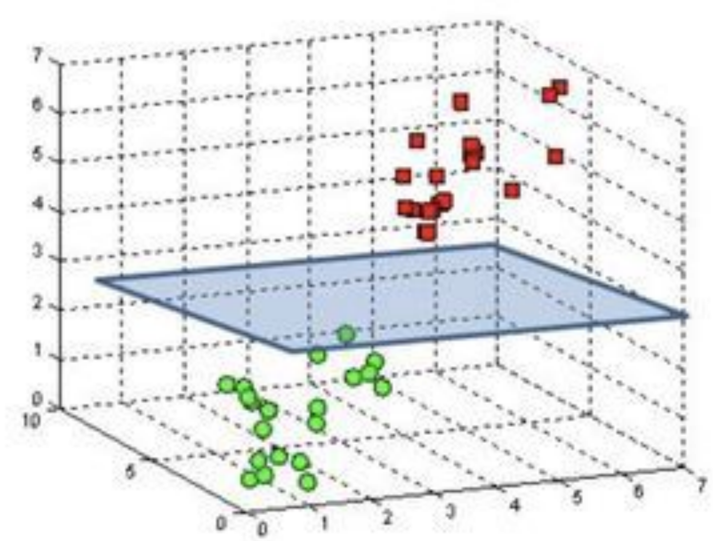


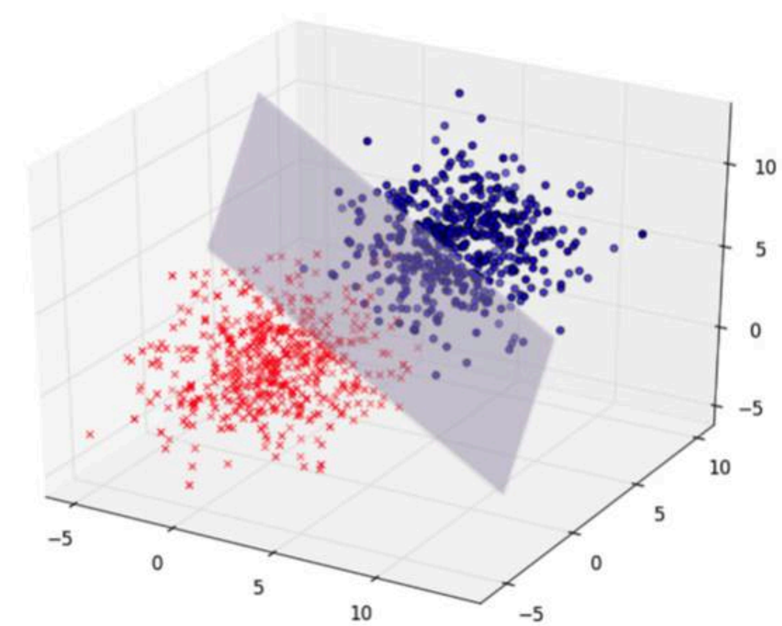


A data point: p-dimensional vector (p=2)
Can be separated by (p-1)-dimensional hyperplane

Hyperplane with maximal margin (largest separation between classes)



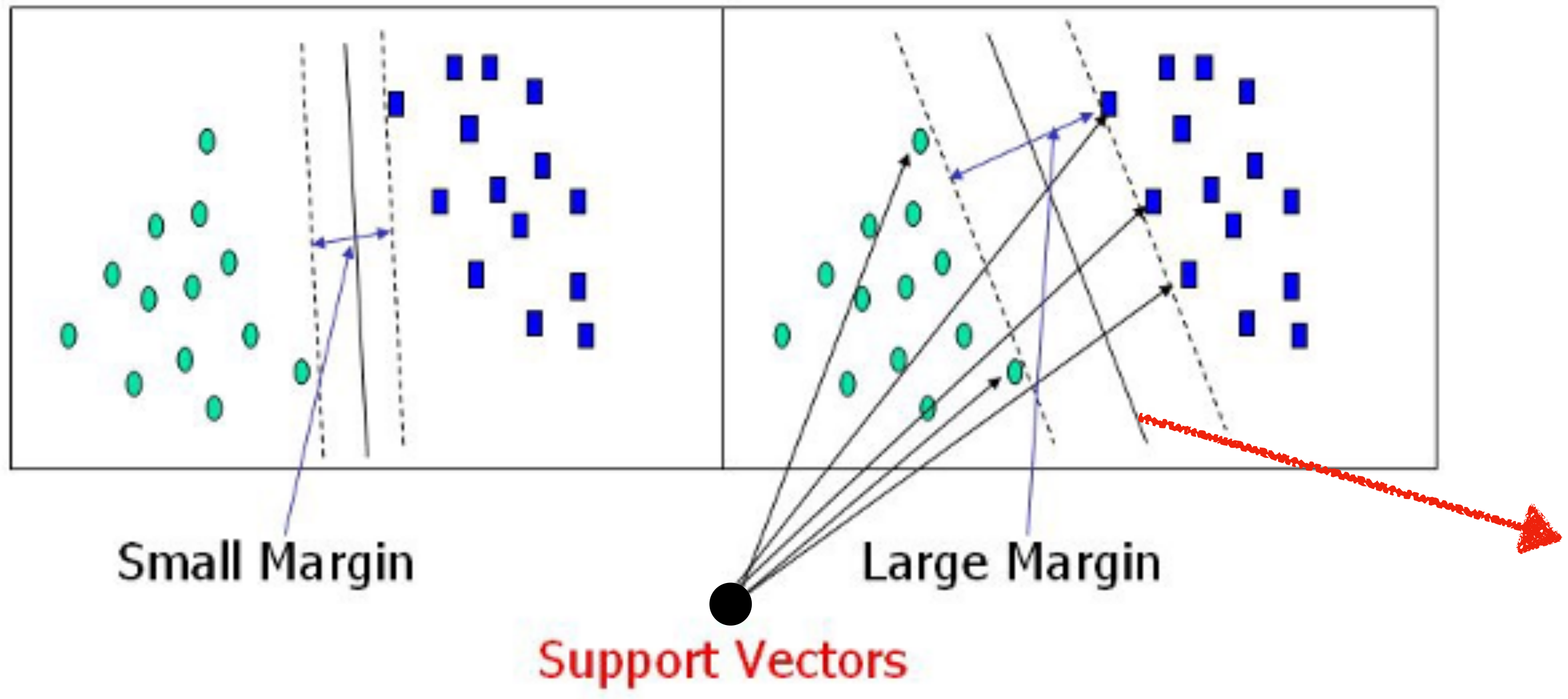




Hyperplane in R^2 is a line

Hyperplane in R^3 is a plane

Support Vector Machine



$$\vec{\omega} \cdot \vec{x}_i + b = 0$$
$$\theta^T \cdot x = 0$$

Optimisation problem with constraints:

Linearly separable training set $$\mathcal{D} = \{(\vec{x}_i, y_i) | \vec{x}_i \in \mathbb{R}^n, y_i \in \{-1, 1\}\}_{i=1}^m$$

Geometric margin $$M = \min_{i=1,2,\cdots,m} \frac{|y_i(\vec{\omega} \cdot \vec{x}_i + b)|}{||\vec{\omega}||}$$

The optimal separating hyperplane is the hyperplane $(\vec{\omega}, b)$ whose margin M is the largest

Some high-school Geometry

Given a plane $w_1 x_1 + w_2 x_2 + b = 0$

* distance from origin $(0,0)$ to the plane is

$$\boxed{\frac{b}{\sqrt{w_1^2 + w_2^2}} = \frac{b}{\|\vec{w}\|}}$$

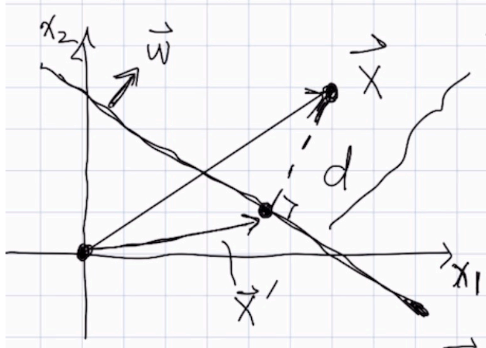
* distance from arbitrary point (x_1, x_2) to the plane is

$$\boxed{\frac{|w_1 x_1 + w_2 x_2 + b|}{\|\vec{w}\|}}$$

* $\vec{w} = (w_1, w_2)$ is the normal vector to the plane

$$\|\vec{w}\| = \sqrt{w_1^2 + w_2^2}$$

Proof of distance from $\vec{x} = (x_1, x_2)$ to the plane $\vec{w} \cdot \vec{x} + b = 0$ $\quad d = \frac{\vec{w} \cdot \vec{x} + b}{\|\vec{w}\|}$



$$\vec{w} \cdot \vec{x} + b = 0$$

$$\vec{X} = \vec{X}' + \hat{d}$$

$$\hat{d} = \frac{\vec{w}}{\|\vec{w}\|} d$$

$$\vec{w} \cdot \vec{x}' + b = 0$$

$$\vec{w} \cdot (\vec{X} - \hat{d}) + b = 0$$

$$\vec{w} \cdot \vec{X} - \vec{w} \cdot \frac{\vec{w}}{\|\vec{w}\|} d + b = 0$$

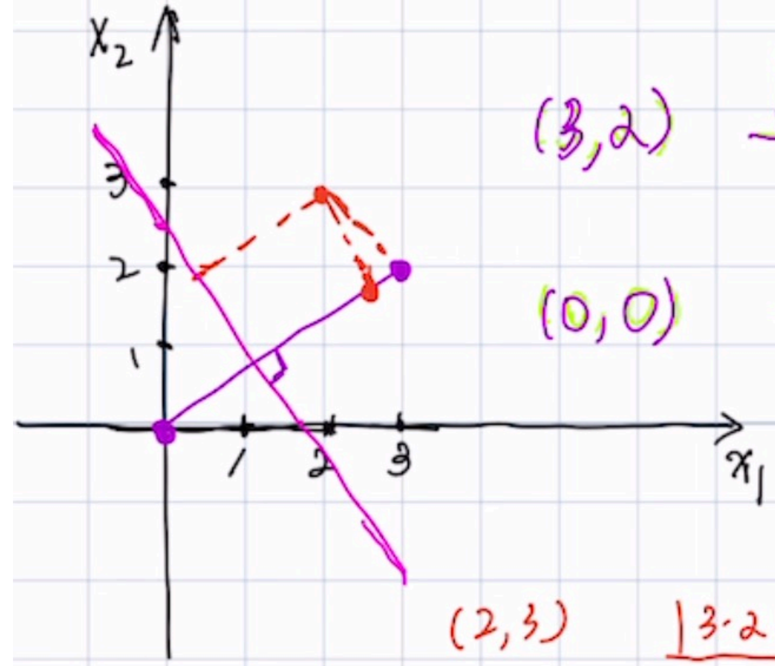
$$d = \frac{\vec{w} \cdot \vec{X} + b}{\|\vec{w}\|}$$

Example

$$3x_1 + 2x_2 - 5 = 0$$

normal vector $\vec{w} = (3, 2)$

$$\|\vec{w}\| = \sqrt{13}$$



$(3,2)$ $\quad \frac{|3 \cdot 3 + 2 \cdot 2 - 5|}{\sqrt{13}} = \frac{8}{\sqrt{13}}$

$(0,0)$ $\quad \frac{|-5|}{\sqrt{13}} = \frac{5}{\sqrt{13}}$

$$\frac{8}{\sqrt{13}} + \frac{5}{\sqrt{13}} = \sqrt{13} = \|\vec{w}\|$$

$(2,3)$ $\quad \frac{|3 \cdot 2 + 2 \cdot 3 - 5|}{\sqrt{13}} = \frac{7}{\sqrt{13}}$

distance between $(2,3)$ and $(3,2)$ $\quad \sqrt{1+1} = \sqrt{2}$

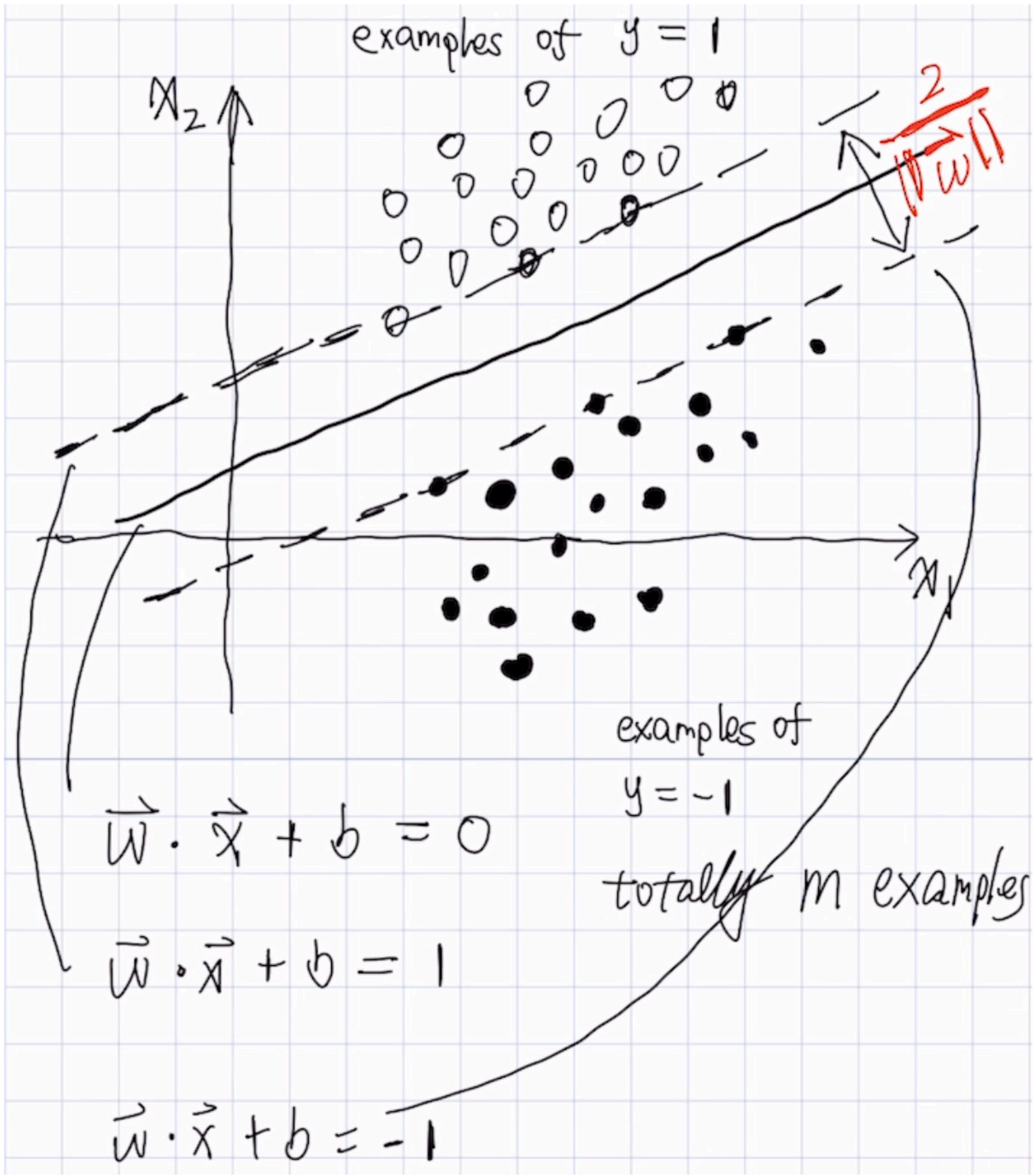
distance between $(2,3)$ and $2x_1 - 3x_2 = 0$ is

$$\frac{|2 \cdot 2 - 3 \cdot 3|}{\sqrt{13}} = \frac{5}{\sqrt{13}}$$

so $\quad \sqrt{2} = \sqrt{\left(\frac{5}{\sqrt{13}}\right)^2 + \left(\frac{1}{\sqrt{13}}\right)^2} = \sqrt{2}$

Support Vector Machine

How to find the optimal hyperplane for a dataset among all possible hyperplanes



Geometric margin M: distance/2 between two hyperplane

$$M = \frac{1}{||\vec{\omega}||}$$

Maximize the geometric margin means minimize

$$||\vec{\omega}||$$

Constraints: at the same time, prevent data points from falling into the margin

To find $(\vec{\omega}, b)$ such that

$$\max_{(\vec{\omega}, b)} M$$

$$\text{subject to} \quad \frac{|y_i(\vec{\omega} \cdot \vec{x}_i + b)|}{||\vec{\omega}||} \geq M, \quad i = 1, 2, \cdots, m$$

Constrained optimization problem

Support Vector Machine

To find $(\vec{\omega}, b)$ such that

$$\max_{(\vec{\omega},b)} M$$

$$\text{subject to} \quad \frac{|y_i(\vec{\omega}\cdot\vec{x}_i + b)|}{||\vec{\omega}||} \geq M, \quad i = 1, 2, \cdots, m$$


PHYSICAL REVIEW X

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Duality between the Deconfined Quantum-Critical Point and the Bosonic Topological Transition

Yan Qi Qin, Yuan-Yao He, Yi-Zhuang You, Zhong-Yi Lu, Arnab Sen, Anders W. Sandvik, Cenke Xu, and Zi Yang Meng

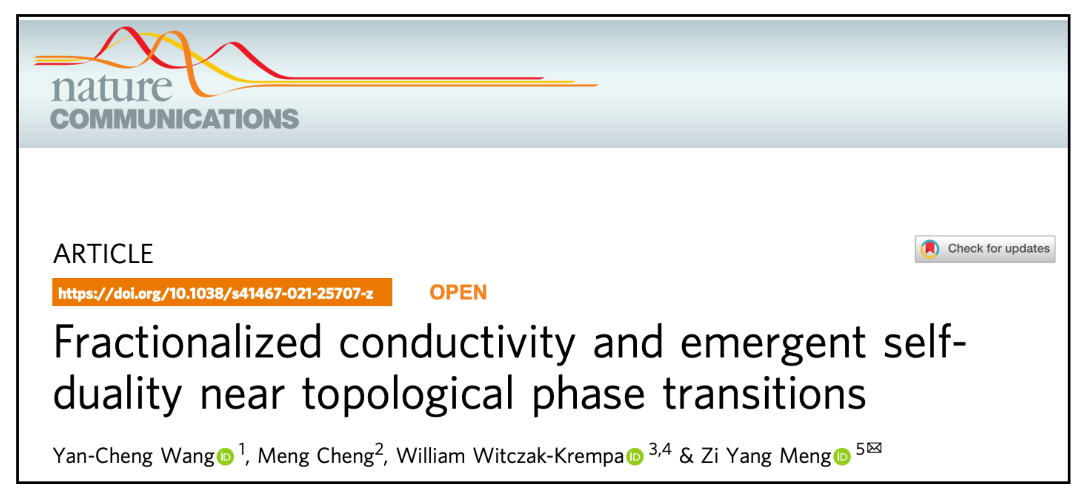
Phys. Rev. X **7**, 031052 – Published 22 September 2017

Is equivalent to the minimisation problem with constraints, remember $M = \dfrac{1}{||\vec{\omega}||}$

$$\min_{(\vec{\omega},b)} ||\vec{\omega}||$$

$$\text{subject to} \quad y_i(\vec{\omega}\cdot\vec{x}_i + b) \geq 1, \; i = 1, 2, \cdots, m$$

Lagrange multipliers and duality


nature COMMUNICATIONS

ARTICLE

Check for updates

https://doi.org/10.1038/s41467-021-25707-z OPEN

Fractionalized conductivity and emergent self-duality near topological phase transitions

Yan-Cheng Wang[1], Meng Cheng[2], William Witczak-Krempa[3,4] & Zi Yang Meng[5]

Is equivalent to

$$\min_{(\vec{\omega},b)} \frac{1}{2}||\vec{\omega}||^2$$

$$\text{subject to} \quad y_i(\vec{\omega}\cdot\vec{x}_i + b) \geq 1, \; i = 1, 2, \cdots, m$$

Convex quadratic optimisation problem

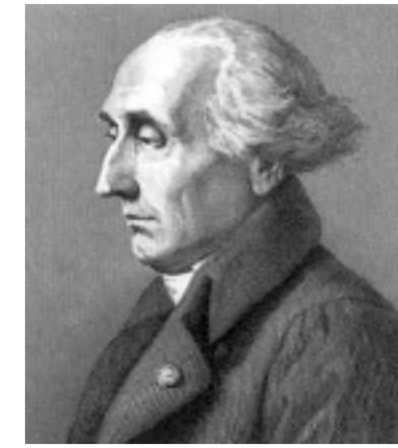
Lagrange multipliers and duality

$$\begin{aligned} \underset{\vec{x}}{\text{minimize}} \quad & f(\vec{x}) \\ \underbrace{\text{subject to} \quad g(\vec{x}) = 0}_{\text{equality constraint}} \end{aligned}$$

$$\mathcal{L} = f(\vec{x}) - \alpha g(\vec{x})$$

find the local maxima and minima

$$\nabla \mathcal{L}(\vec{x}, \alpha) = \nabla f(\vec{x}) - \alpha \nabla g(\vec{x}) = 0$$



Joseph-Louis Lagrange (1736-1813)

"I will deduce the complete mechanics of solid and fluid bodies using the principle of least action."

JOSEPH-LOUIS LAGRANGE

Letter to Leonhard Euler, May 1756

"I have almost completed a book on analytical mechanics founded solely on the principle [of virtual work]. But since I still have no idea where and when it can be published, I am not in any hurry to finish it."

JOSEPH-LOUIS LAGRANGE

Letter to Pierre Laplace, September 1782

$$\underset{x,y}{\text{minimize}} \quad f(x,y) = x^2 + y^2$$
$$\text{subject to} \quad g(x,y) = x + y - 1 = 0$$

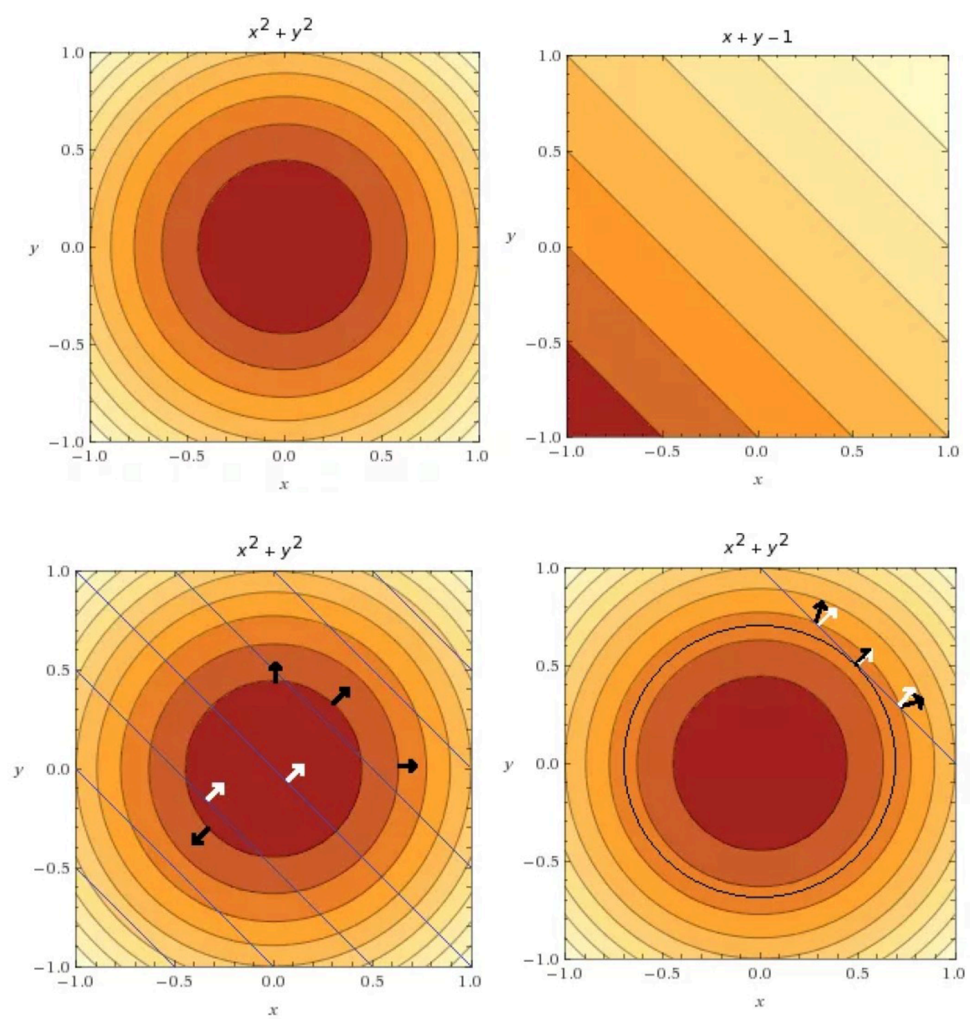
$$\mathcal{L}(x,y,\alpha) = f(x,y) - \alpha g(x,y)$$

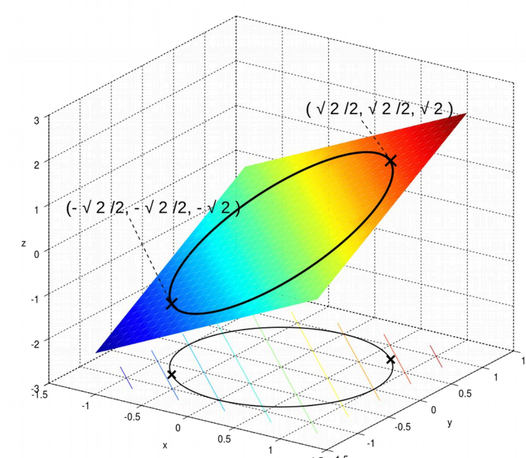
$$\nabla \mathcal{L}(x,y,\alpha) = \nabla f(x,y) - \alpha \nabla g(x,y) = 0$$

$$\nabla_{x_1,x_2,\cdots,x_n,\alpha} \mathcal{L}(x_1,x_2,\cdots,x_n,\alpha) = 0$$

$$\frac{\partial \mathcal{L}}{\partial x} = 0 \qquad \frac{\partial \mathcal{L}}{\partial y} = 0 \qquad \frac{\partial \mathcal{L}}{\partial \alpha} = 0$$

$$x = y = \frac{1}{2} \qquad \alpha = 1$$

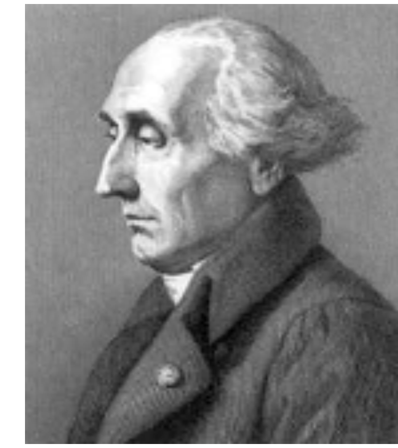




$$f(x,y) = x + y$$

$$g(x,y) = x^2 + y^2 - 1 = 0$$

Lagrange multipliers and duality



Joseph-Louis Lagrange (1736-1813)

$$\underset{\vec{x}}{\text{minimize}} \quad f(\vec{x})$$
$$\underbrace{\text{subject to} \quad g(\vec{x}) = 0}_{\text{equality constraint}}$$

$$\mathcal{L} = f(\vec{x}) - \alpha g(\vec{x})$$

$$\nabla \mathcal{L}(\vec{x}, \alpha) = \nabla f(\vec{x}) - \alpha \nabla g(\vec{x}) = 0$$

"I will deduce the complete mechanics of solid and fluid bodies using the principle of least action."

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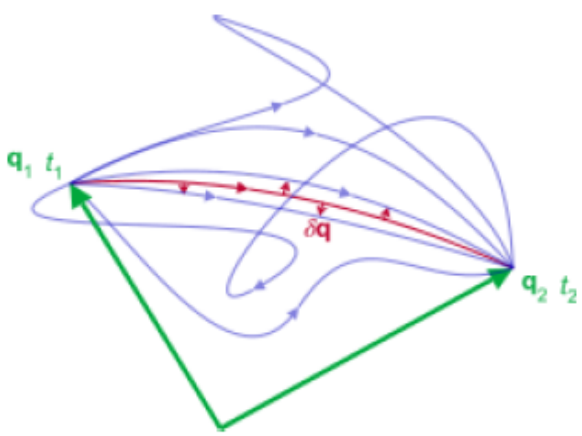
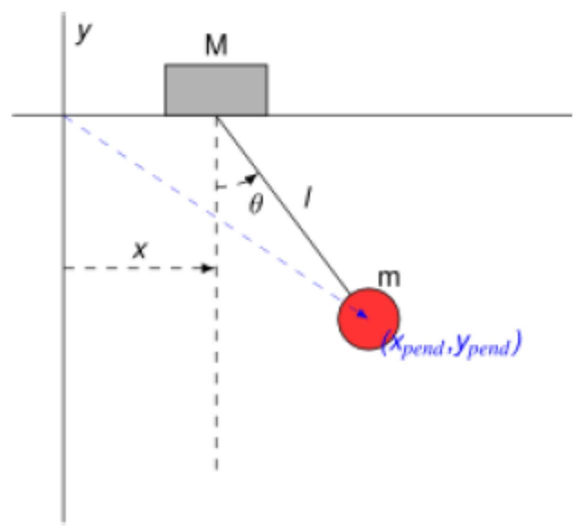
$$L = T - V$$

Euler-Lagrange equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}_j}\right) = \frac{\partial L}{\partial q_j}$$



As the system evolves, **q** traces a path through configuration space (only some are shown). The path taken by the system (red) has a stationary action (δS = 0) under small changes in the configuration of the system (δ**q**).[27]



Sketch of the situation with definition of the coordinates (click to enlarge)

$$T = \frac{1}{2}M\dot{x}^2 + \frac{1}{2}m\left(\dot{x}_{\text{pend}}^2 + \dot{y}_{\text{pend}}^2\right)$$

$$V = mgy_{\text{pend}}$$

$$\begin{aligned} L &= T - V \\ &= \tfrac{1}{2}M\dot{x}^2 + \tfrac{1}{2}m\left[\left(\dot{x} + \ell\dot{\theta}\cos\theta\right)^2 + \left(\ell\dot{\theta}\sin\theta\right)^2\right] + mg\ell\cos\theta \end{aligned}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[m(\dot{x}\ell\cos\theta + \ell^2\dot{\theta})\right] + m\ell(\dot{x}\dot{\theta} + g)\sin\theta = 0$$

$$\ddot{\theta} + \frac{\ddot{x}}{\ell}\cos\theta + \frac{g}{\ell}\sin\theta = 0$$

$$S = \int_{t_1}^{t_2} L\,\mathrm{d}t\,, \qquad \delta S = 0$$

principle of least action

Lagrange multipliers and duality

$$\min_{(\vec{\omega},b)} \frac{1}{2}||\vec{\omega}||^2$$

$$\text{subject to} \quad y_i(\vec{\omega}\cdot\vec{x}_i + b) \geq 1,\ i = 1, 2, \cdots, m$$

$$\mathscr{L}(\overrightarrow{\omega}, b, \alpha) = \frac{1}{2}||\overrightarrow{\omega}||^2 - \sum_{i=1}^{m} \alpha_i[y_i(\overrightarrow{\omega}\cdot\overrightarrow{x}_i + b) - 1]$$

$$\min_{(\vec{\omega},b)} \max_{\alpha} \mathcal{L}(\vec{\omega}, b, \alpha)$$

$$\text{subject to} \quad \alpha_i \geq 0, i = 1, 2, \cdots, m$$

$$\nabla_{\vec{\omega}}\mathcal{L} = \vec{\omega} - \sum_{i=1}^{m} \alpha_i y_i \vec{x}_i = 0$$

$$\frac{\partial \mathcal{L}}{\partial b} = -\sum_{i=1}^{m} \alpha_i y_i = 0$$

$$\mathcal{L}_D = \sum_{i=1}^{m} \alpha_i - \frac{1}{2}\sum_{i=1}^{m}\sum_{j=1}^{m} \alpha_i\alpha_j y_i y_j \vec{x}_i\cdot\vec{x}_j$$

$$\max_{\alpha} \mathcal{L}_D(\alpha, \vec{x}_i, y_i)$$

$$\text{subject to} \quad \alpha_i \geq 0, i = 1, 2, \cdots, m$$

$$\sum_{i=1}^{m} \alpha_i y_i = 0$$

gradient, not the -gradient

Karush-Kuhn-Tucker (KKT) conditions

- Stationarity condition:

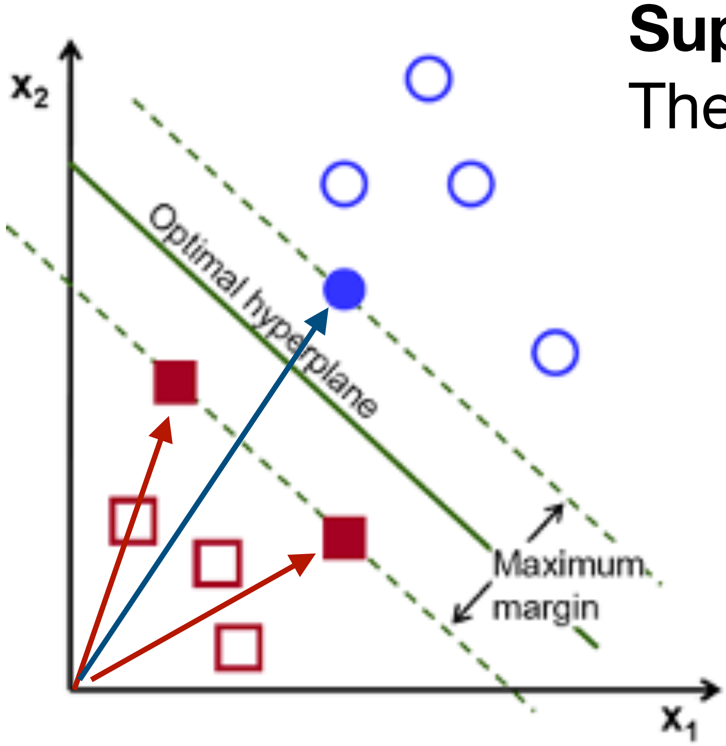
$$\nabla_{\vec{\omega}}\mathcal{L} = \vec{\omega} - \sum_{i=1}^{m} \alpha_i y_i \vec{x}_i = 0$$

$$\frac{\partial \mathcal{L}}{\partial b} = -\sum_{i=1}^{m} \alpha_i y_i = 0$$

- Primal feasibility condition: $y_i(\vec{\omega}\cdot\vec{x}_i + b) - 1 \geq 0 \quad \text{for all } i = 1, 2, \cdots, m$

- Dual feasibility condition: $\alpha_i \geq 0 \quad \text{for all } i = 1, 2, \cdots, m$

- Complementary slackness condition: $\alpha_i[y_i(\vec{\omega}\cdot\vec{x}_i + b) - 1] = 0 \quad \text{for all } i = 1, 2, \cdots, m$



Support vectors are examples having a positive Lagrange multiplier. They are the ones the constraint is active.

Once have the multipliers and support vectors

$$\vec{\omega} = \sum_{i=1}^{m} \alpha_i y_i \vec{x}_i$$

$$b = \frac{1}{S}\sum_{i=1}^{S}(y_i - \vec{\omega}\cdot\vec{x}_i)$$

S is the number of support vectors

Support Vector Machine: Hinge Loss

$$\mathscr{L}(\overrightarrow{\omega}, b, \alpha) = \frac{1}{2}||\overrightarrow{\omega}||^2 - \sum_{i=1}^{m} \alpha_i[y_i(\overrightarrow{\omega} \cdot \overrightarrow{x}_i + b) - 1]$$

$$J(\overrightarrow{\omega}, b) = \frac{1}{2m}||\overrightarrow{\omega}||^2 + \frac{1}{m}\sum_{i=1}^{m} \max(0,1 - y_i(\overrightarrow{\omega} \cdot \overrightarrow{x}_i + b))$$

Replace $\frac{1}{2m}$ with $\frac{\lambda}{2m}$ for regularisation

$y_i = 1$

$\vec{\omega} \cdot \vec{x}_i + b > 1$ $\quad \nabla_{\overrightarrow{\omega}} J = \frac{1}{m}\overrightarrow{\omega}$

$\vec{\omega} \cdot \vec{x}_i + b < 1$ $\quad \nabla_{\overrightarrow{\omega}} J = \frac{1}{m}\overrightarrow{\omega} - y_i\overrightarrow{x}_i$

$\nabla_b J = - y_i$

$y_i = -1$

$\vec{\omega} \cdot \vec{x}_i + b < -1$ $\quad \nabla_{\overrightarrow{\omega}} J = \frac{1}{m}\overrightarrow{\omega}$

$\vec{\omega} \cdot \vec{x}_i + b > -1$ $\quad \nabla_{\overrightarrow{\omega}} J = \frac{1}{m}\overrightarrow{\omega} - y_i\overrightarrow{x}_i$

$\nabla_b J = - y_i$

Gradient Descent

$$\vec{\omega} = \vec{\omega} - \alpha \nabla_{\vec{\omega}} J$$

$$b = b - \alpha \nabla_b J$$

Support Vector Machine: Hinge Loss

$$J(\theta) = -\frac{1}{M}\sum_{i=1}^{M}\left[y^{(i)}\log h_\theta(x^{(i)}) + (1-y^{(i)})\log(1-h_\theta(x^{(i)}))\right]$$

$$J(\theta) = \frac{1}{M}\sum_{i=1}^{M}\max(0,\ 1-y_i(\vec{\theta}\cdot\vec{x}_i+\theta_0))$$

Hinge function

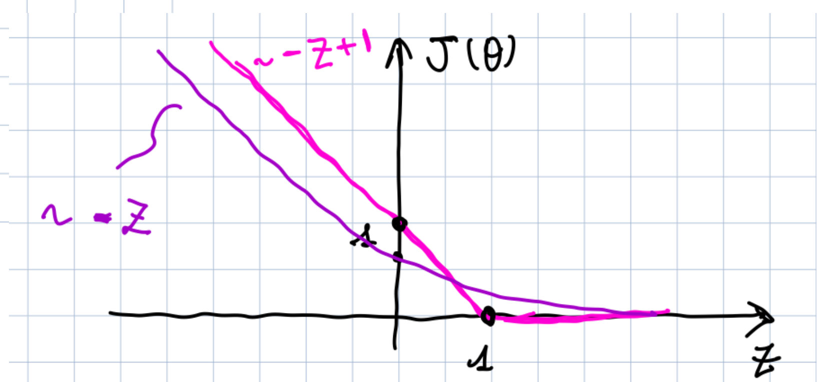
$y_i = 1 \quad \vec{\theta}\cdot\vec{x}_i + \theta_0 \geq 1 \quad J(\theta) = 0$

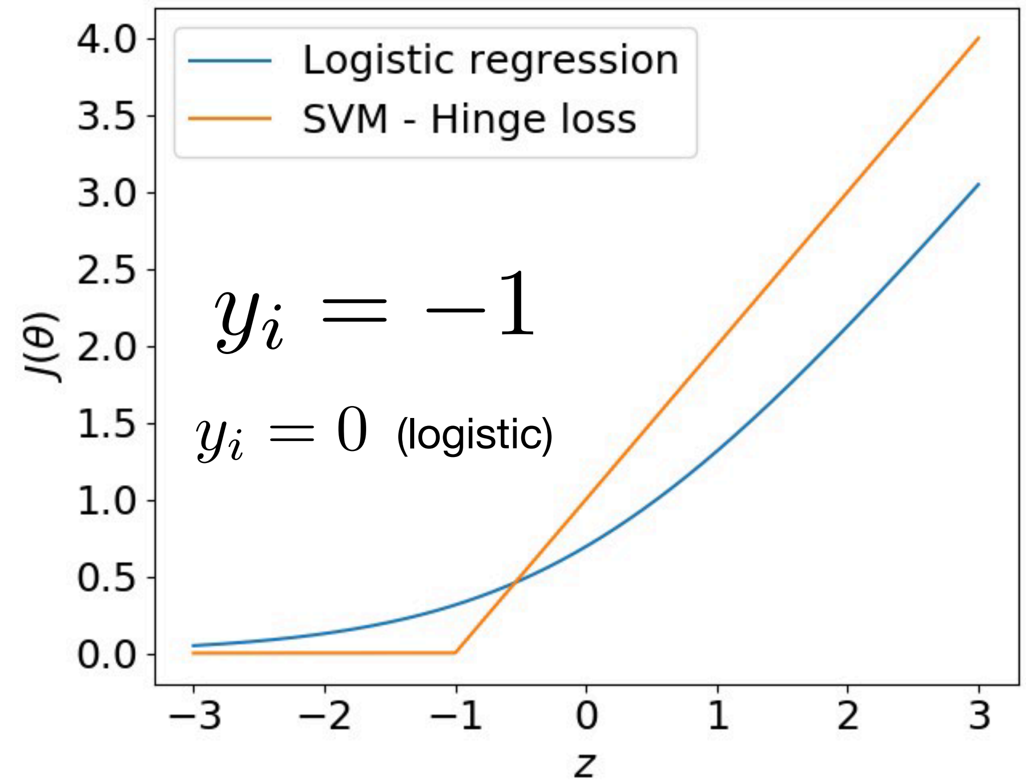
$\quad\quad\quad \vec{\theta}\cdot\vec{x}_i + \theta_0 < 1 \quad J(\theta) = 1-(\vec{\theta}\cdot\vec{x}_i+\theta_0)$

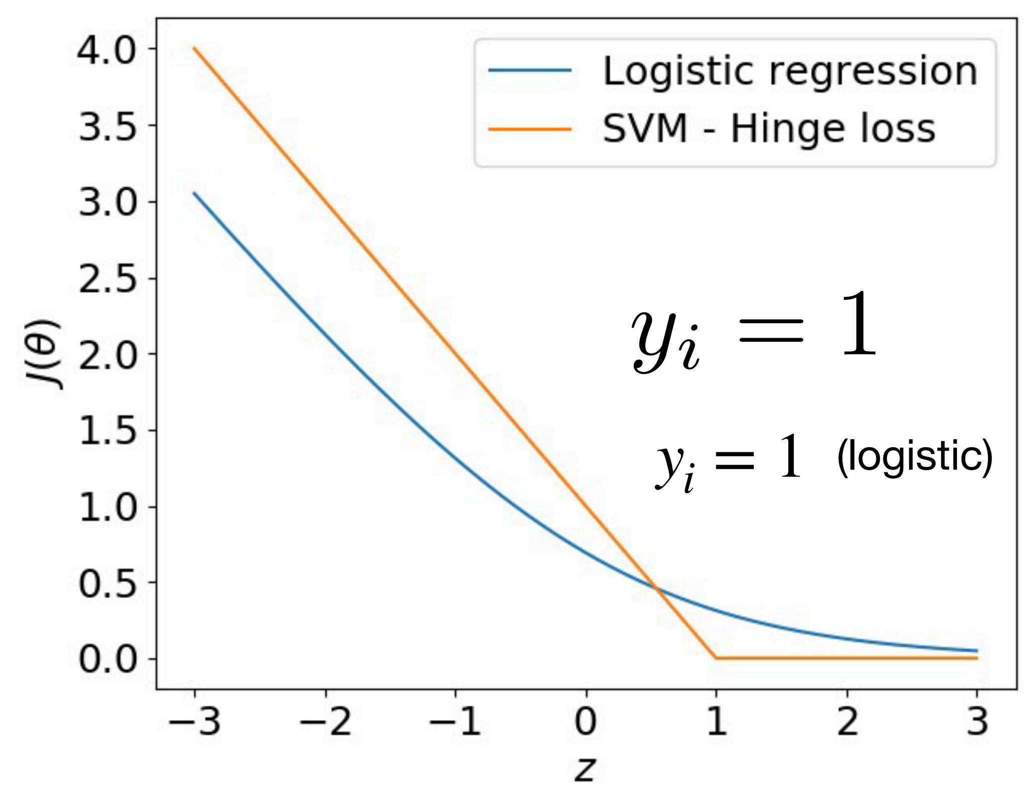
remember in logistic regression

$$J(\theta) = -\log\frac{1}{1+e^{-\theta\cdot x}}$$

$$z = \theta\cdot x = \vec{\theta}\cdot\vec{x} + \theta_0$$

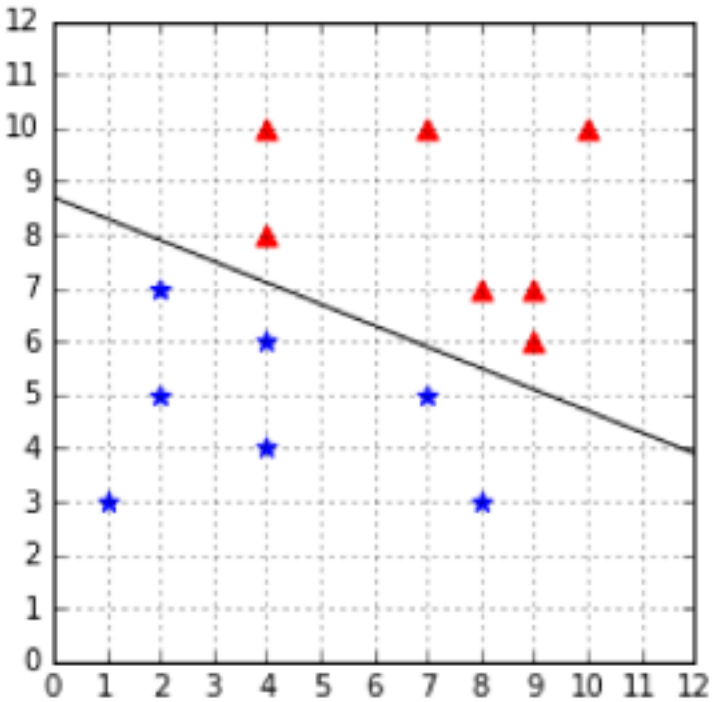




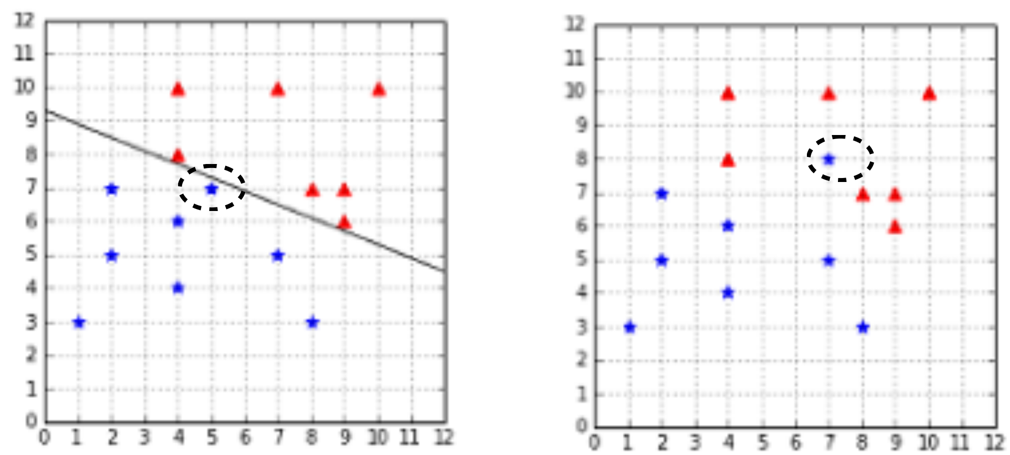


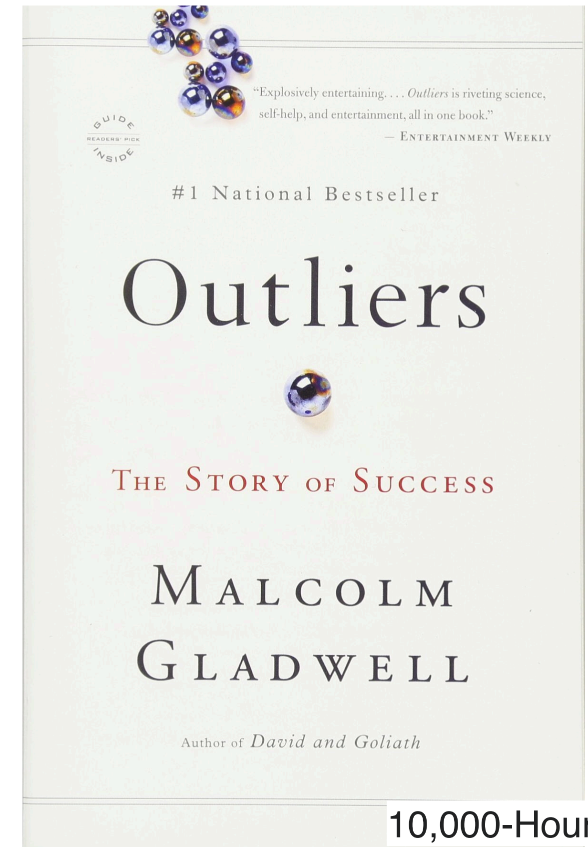
Support Vector Machine: hard margin and soft margin

Linearly separable



Outliers





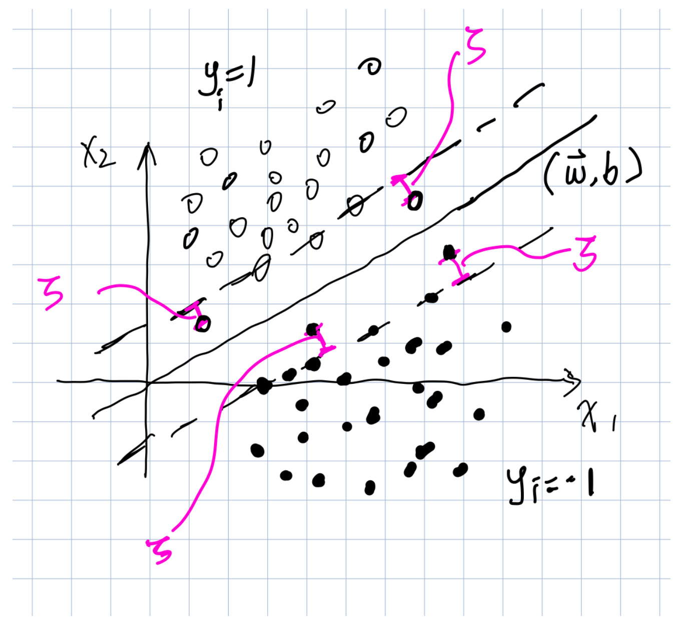
10,000-Hour Rule

Soft margin to rescue

$$y_i(\vec{\omega} \cdot \vec{x}_i + b) \geq 1$$

$$y_i(\vec{x} \cdot \vec{x}_i + b) \geq 1 - \zeta_i$$

slack variables



Modify the objective function with regularization

$$\underset{(\vec{\omega},b,\zeta)}{\text{minimize}} \quad \frac{1}{2}||\vec{\omega}||^2 + C\sum_{i=1}^{m}\zeta_i$$

$$\text{subject to} \;\; y_i(\vec{\omega} \cdot \vec{x}_i + b) \geq 1 - \zeta_i$$

$$\zeta_i \geq 0 \;\; \text{for any } i = 1, \cdots, m$$

Lagrange multipliers and duality

$$\mathcal{L}(\vec{\omega}, b, \alpha, \zeta) = \frac{1}{2}||\vec{\omega}||^2 + C\sum_{i=1}^{m}\zeta_i - \sum_{i=1}^{m}\alpha_i\left[y_i(\vec{\omega}_i \cdot \vec{x}_i + b) - 1 + \zeta_i\right]$$

$$\nabla_{\vec{\omega}}\mathcal{L} = \vec{\omega} - \sum_{i=1}^{m}\alpha_i y_i \vec{x}_i = 0$$

Karush-Kuhn-Tucker (KKT) conditions

$$\frac{\partial \mathcal{L}}{\partial b} = -\sum_{i=1}^{m}\alpha_i y_i = 0$$

$$\frac{\partial \mathcal{L}}{\partial \zeta} = C - \alpha = 0$$

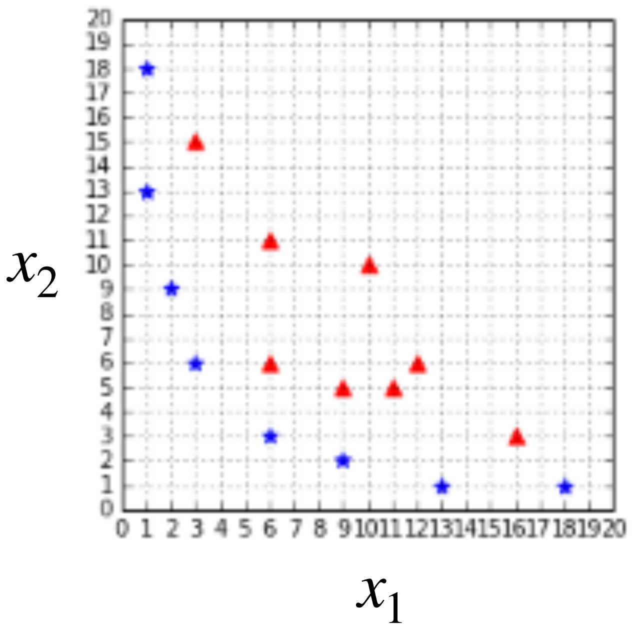
$$\mathcal{L}_D = \sum_{i=1}^{m}\alpha_i - \frac{1}{2}\sum_{i=1}^{m}\sum_{j=1}^{m}\alpha_i\alpha_j y_i y_j \vec{x}_i \cdot \vec{x}_j$$

$$\max_{\alpha} \mathcal{L}_D(\alpha, \vec{x}_i, y_i)$$

$$\text{subject to} \quad 0 \leq \alpha_i \leq C, \quad i = 1, 2, \cdots, m$$

$$\sum_{i=1}^{m}\alpha_i y_i = 0$$

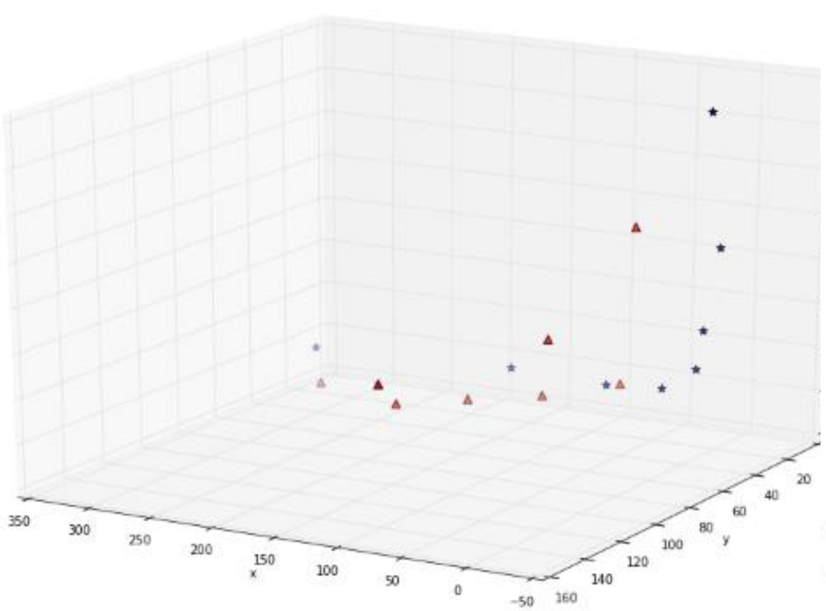
Kernel machine: Dimensionality reduction strike

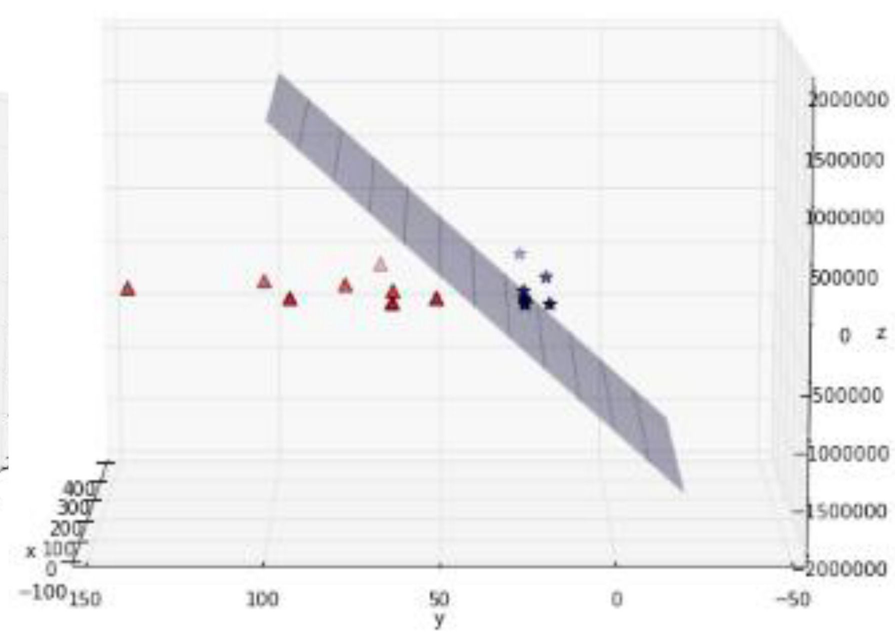


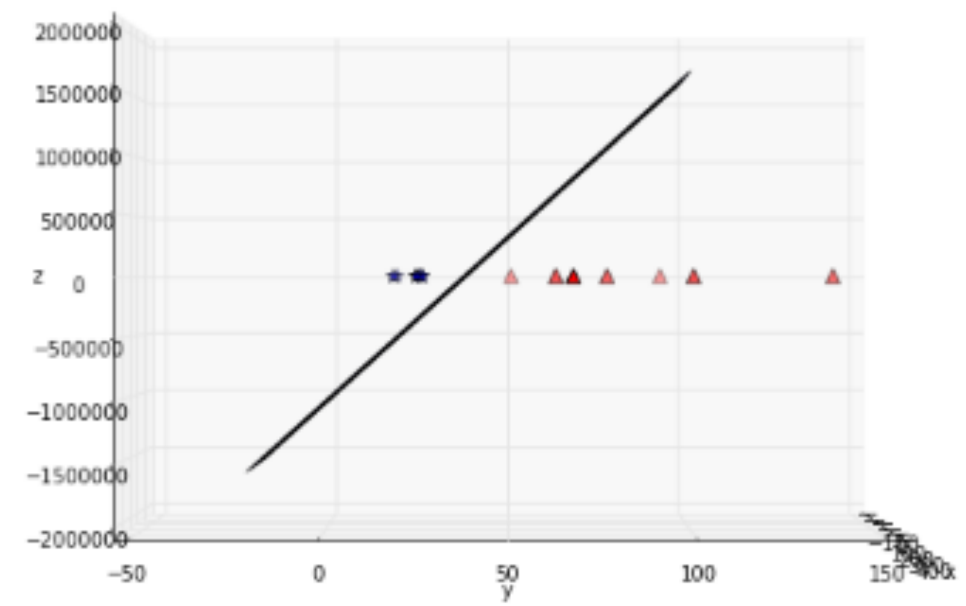
Not linearly separable in **two dimensions**

Polynomial mapping $\phi : \mathbb{R}^2 \rightarrow \mathbb{R}^3$ $\phi(x_1, x_2) = (x_1^2, \sqrt{2}x_1x_2, x_2^2)$

$$\begin{aligned}\langle \phi(\vec{x}_i), \phi(\vec{x}_j) \rangle_{\mathbb{R}^3} &= (x_{i,1}^2, \sqrt{2}x_{i,1}x_{i,2}, x_{i,2}^2) \cdot (x_{j,1}^2, \sqrt{2}x_{j,1}x_{j,2}, x_{j,2}^2) \\ &= x_{i,1}^2 x_{i,2}^2 + 2x_{i,1}x_{i,2}x_{j,1}x_{j,2} + x_{i,2}^2 x_{j,2}^2 \\ &= (\vec{x}_i \cdot \vec{x}_j + c)^d \quad \text{with } c = 0 \text{ and } d = 2\end{aligned}$$







Kernel machine: Dimensionality reduction strike

mapping $\phi : \mathcal{X} \rightarrow \mathcal{V}$

function $K : \mathcal{X} \rightarrow \mathbb{R}$ $\quad K(\vec{x}, \vec{x}') = \langle \phi(\vec{x}), \phi(\vec{x}') \rangle_{\mathcal{V}}$

inner production in $\mathcal{V}$, **kernel function**

$$\max_{\alpha} \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_i \alpha_j y_i y_j K(\vec{x}_i, \vec{x}_j)$$

subject to $0 \leq \alpha_i \leq C, \; i = 1, \cdots, m$

$$\sum_{i=1}^{m} \alpha_i y_i = 0$$

$$K(\vec{x}, \vec{x}') = (\vec{x} \cdot \vec{x}' + c)^d$$

$c = 1, d = 1$ linear kernel

$c = 0, d = 2$ quadratic kernel