Math for ML

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Probability for Machine learning

A random variable is a real-valued function defined on the set of outcomes of a random experiment.

A process that has random outcomes is called a random experiment

The set of all possible outcomes of a random experiment is called the sample space and is denoted Ω.

A combination of outcomes, a subset of Ω, is called an event.

The set of events is denoted A. It is assumed that the set A is a σ-algebra which means that the following properties hold for A:

(a) $\Omega \in \mathcal{A}$

(b) $A^c \in \mathcal{A}$ if $A \in \mathcal{A}$, where A^c is the complement of set A

(c) $\cup_{i=1}^{\infty} A_i \in \mathcal{A}$ if $A_1, A_2, \cdots \in \mathcal{A}$.

The probability P is a set function that maps A into [0, 1] and P is called a probability measure if the following conditions hold:

(d) $P(\Omega) = 1$

(e) $P(A^c) = 1 - P(A)$

(f) $P(\cup_{i=1}^{n} A_i) = \sum_{i=1}^{n} P(A_i), \quad \text{if} \quad A_i \cap A_j = \phi \quad \text{for} \quad i \neq j.$

Example

Flipping a coin twice; generating a σ-algebra set

Number of observations; Poisson distributed

$$P_0(t+\Delta t) = (1-\lambda\Delta t)P_0(t) + o(\Delta t)$$

$$P_n(t+\Delta t) = (1-\lambda\Delta t)P_n(t) + \lambda\Delta t P_{n-1}(t) + o(\Delta t)$$

$$\frac{dP_0(t)}{dt} = -\lambda P_0(t), \quad P_0(0) = 1$$

$$\frac{dP_n(t)}{dt} = -\lambda P_n(t) + \lambda P_{n-1}(t), \quad P_n(0) = 1, \quad \text{for} \quad n \geq 1.$$

$$P(\{\omega_n\}) = P_n(t) = \exp(-\lambda t)(\lambda t)^n/n!$$

A random variable X is a real-valued function that assigns the value $X(\omega) \in R$ to each outcome $\omega \in \Omega$. That is, $X : \Omega \rightarrow R$. The function $F(x) = P(\{\omega \in \Omega : X(\omega) \leq x\})$ is called the distribution function or the probability distribution of the random variable X.

$$E(X) = \int_{-\infty}^{\infty} xp(x)\,dx.$$

$$E(g(X)) = \int_{-\infty}^{\infty} g(x)p(x)\,dx.$$

$$E(X^k) = \int_{-\infty}^{\infty} x^k p(x)\,dx.$$

Sum rule

$$p(\boldsymbol{x}) = \begin{cases} \sum_{\boldsymbol{y} \in \mathcal{Y}} p(\boldsymbol{x}, \boldsymbol{y}) & \text{if } \boldsymbol{y} \text{ is discrete} \\ \int_{\mathcal{Y}} p(\boldsymbol{x}, \boldsymbol{y}) \mathrm{d}\boldsymbol{y} & \text{if } \boldsymbol{y} \text{ is continuous} \end{cases},$$

Product rule

$$p(\boldsymbol{x}, \boldsymbol{y}) = p(\boldsymbol{y} \mid \boldsymbol{x}) p(\boldsymbol{x}) \, .$$

Bayes rule

$$\underbrace{p(\boldsymbol{x} \mid \boldsymbol{y})}_{\text{posterior}} = \frac{\overbrace{p(\boldsymbol{y} \mid \boldsymbol{x})}^{\text{likelihood}} \overbrace{p(\boldsymbol{x})}^{\text{prior}}}{\underbrace{p(\boldsymbol{y})}_{\text{evidence}}}$$

Marginal probability

$$p(\boldsymbol{y}) := \int p(\boldsymbol{y} \mid \boldsymbol{x}) p(\boldsymbol{x}) \mathrm{d}\boldsymbol{x} = \mathbb{E}_X[p(\boldsymbol{y} \mid \boldsymbol{x})]$$

$$P(C_i|\boldsymbol{X}) = \frac{P(\boldsymbol{X}|C_i)P(C_i)}{P(\boldsymbol{X})}.$$

$$P(\boldsymbol{X}|C_i) = \prod_{k=1}^{n} P(x_k|C_i)$$
$$= P(x_1|C_i) \times P(x_2|C_i) \times \cdots \times P(x_n|C_i).$$

age	income	student	credit_rating	comp
<=30	high	no	fair	no
<=30	high	no	excellent	no
31…40	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
>40	low	yes	excellent	no
31…40	low	yes	excellent	yes
<=30	medium	no	fair	no
<=30	low	yes	fair	yes
>40	medium	yes	fair	yes
<=30	medium	yes	excellent	yes
31…40	medium	no	excellent	yes
31…40	high	yes	fair	yes
>40	medium	no	excellent	no

$$\boldsymbol{X} = (age = youth, income = medium, student = yes, credit\_rating = fair)$$

$$P(\boldsymbol{X}|C_i)P(C_i), \text{ for } i = 1, 2.$$

$$P(buys\_computer = yes) = 9/14 = 0.643$$
$$P(buys\_computer = no) = 5/14 = 0.357$$

$$P(age = youth \mid buys\_computer = yes) = 2/9 = 0.222$$
$$P(age = youth \mid buys\_computer = no) = 3/5 = 0.600$$
$$P(income = medium \mid buys\_computer = yes) = 4/9 = 0.444$$
$$P(income = medium \mid buys\_computer = no) = 2/5 = 0.400$$
$$P(student = yes \mid buys\_computer = yes) = 6/9 = 0.667$$

$$P(student = yes \mid buys\_computer = no) = 1/5 = 0.200$$
$$P(credit\_rating = fair \mid buys\_computer = yes) = 6/9 = 0.667$$
$$P(credit\_rating = fair \mid buys\_computer = no) = 2/5 = 0.400$$

$$
\begin{aligned}
P(\boldsymbol{X}|buys\_computer = yes) = {} & P(age = youth \mid buys\_computer = yes) \\
& \times P(income = medium \mid buys\_computer = yes) \\
& \times P(student = yes \mid buys\_computer = yes) \\
& \times P(credit\_rating = fair \mid buys\_computer = yes) \\
= {} & 0.222 \times 0.444 \times 0.667 \times 0.667 = 0.044.
\end{aligned}
$$

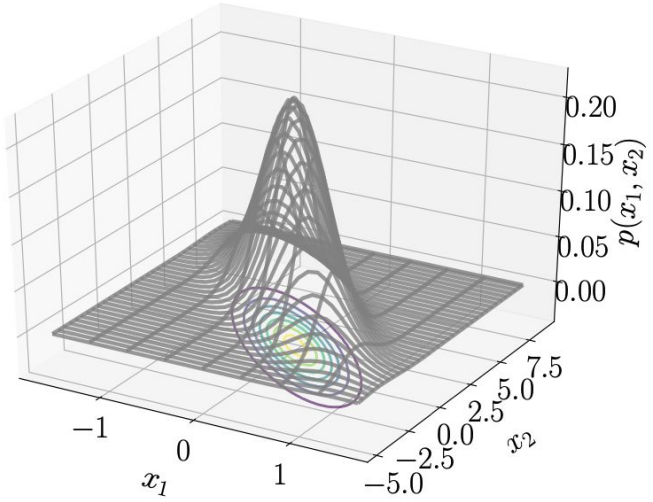
$$
P(\boldsymbol{X}|buys\_computer = no) = 0.600 \times 0.400 \times 0.200 \times 0.400 = 0.019.
$$

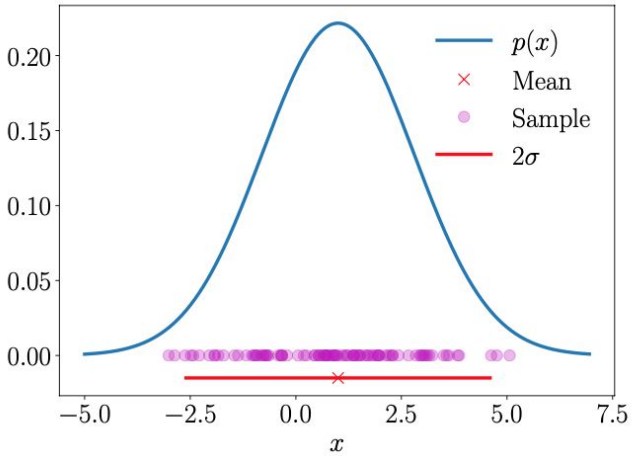
$$P(\boldsymbol{X}|buys\_computer = yes)P(buys\_computer = yes) = 0.044 \times 0.643 = 0.028$$
$$P(\boldsymbol{X}|buys\_computer = no)P(buys\_computer = no) = 0.019 \times 0.357 = 0.007$$

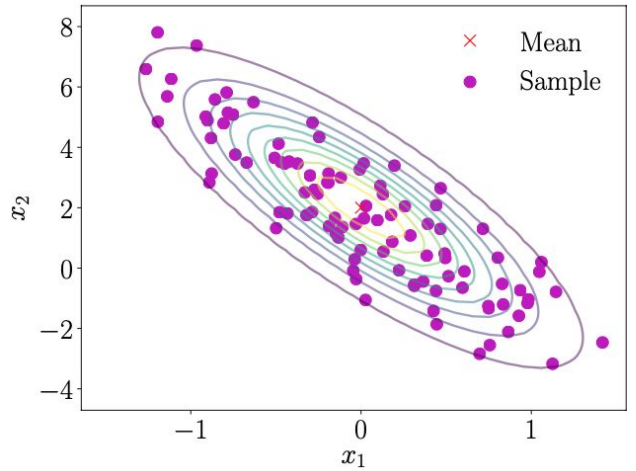
independence

$$p(\boldsymbol{x}, \boldsymbol{y}) = p(\boldsymbol{x})p(\boldsymbol{y})\,.$$

- $p(\boldsymbol{y} \mid \boldsymbol{x}) = p(\boldsymbol{y})$
- $p(\boldsymbol{x} \mid \boldsymbol{y}) = p(\boldsymbol{x})$
- $\mathbb{V}_{X,Y}[\boldsymbol{x} + \boldsymbol{y}] = \mathbb{V}_X[\boldsymbol{x}] + \mathbb{V}_Y[\boldsymbol{y}]$
- $\mathrm{Cov}_{X,Y}[\boldsymbol{x}, \boldsymbol{y}] = \mathbf{0}$


0.20
0.15
0.10
0.05
0.00
$p(x_1, x_2)$
−1
0
1
x_1
7.5
5.0
2.5
0.0
−2.5
−5.0
x_2


0.20
0.15
0.10
0.05
0.00
$p(x)$
Mean
Sample
2σ
−5.0
−2.5
0.0
2.5
5.0
7.5
x


8
6
4
2
0
−2
−4
x_2
Mean
Sample
−1
0
1
x_1

Normal distribution

$$p(x \mid \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right).$$

$$p(\boldsymbol{x} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma}) = (2\pi)^{-\frac{D}{2}} |\boldsymbol{\Sigma}|^{-\frac{1}{2}} \exp\left(-\tfrac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu})\right),$$

$$p(\boldsymbol{x}, \boldsymbol{y}) = \mathcal{N}\left(\begin{bmatrix} \boldsymbol{\mu}_x \\ \boldsymbol{\mu}_y \end{bmatrix}, \begin{bmatrix} \boldsymbol{\Sigma}_{xx} & \boldsymbol{\Sigma}_{xy} \\ \boldsymbol{\Sigma}_{yx} & \boldsymbol{\Sigma}_{yy} \end{bmatrix} \right).$$

$$p(\boldsymbol{x} \mid \boldsymbol{y}) = \mathcal{N}\left(\boldsymbol{\mu}_{x \mid y}, \boldsymbol{\Sigma}_{x \mid y}\right)$$

$$\boldsymbol{\mu}_{x \mid y} = \boldsymbol{\mu}_x + \boldsymbol{\Sigma}_{xy} \boldsymbol{\Sigma}_{yy}^{-1} (\boldsymbol{y} - \boldsymbol{\mu}_y)$$

$$\boldsymbol{\Sigma}_{x \mid y} = \boldsymbol{\Sigma}_{xx} - \boldsymbol{\Sigma}_{xy} \boldsymbol{\Sigma}_{yy}^{-1} \boldsymbol{\Sigma}_{yx}.$$

$$p(\boldsymbol{x}) = \int p(\boldsymbol{x}, \boldsymbol{y}) d\boldsymbol{y} = \mathcal{N}\left(\boldsymbol{x} \,|\, \boldsymbol{\mu}_x,\, \boldsymbol{\Sigma}_{xx}\right).$$

$$p(y \mid \boldsymbol{x}) = \mathcal{N}\left(y \mid f(\boldsymbol{x}),\, \sigma^2\right) .$$

$$y = f(\boldsymbol{x}) + \epsilon \,,$$

$$p(y \mid \boldsymbol{x}, \boldsymbol{\theta}) = \mathcal{N}\left(y \mid \boldsymbol{x}^\top \boldsymbol{\theta},\, \sigma^2\right)$$
$$\iff y = \boldsymbol{x}^\top \boldsymbol{\theta} + \epsilon \,, \quad \epsilon \sim \mathcal{N}\left(0,\, \sigma^2\right) ,$$

$$
\begin{aligned}
p(\mathcal{Y} \mid \mathcal{X}, \boldsymbol{\theta}) &= p(y_1, \ldots, y_N \mid \boldsymbol{x}_1, \ldots, \boldsymbol{x}_N, \boldsymbol{\theta}) \\
&= \prod_{n=1}^{N} p(y_n \mid \boldsymbol{x}_n, \boldsymbol{\theta}) = \prod_{n=1}^{N} \mathcal{N}\left(y_n \mid \boldsymbol{x}_n^\top \boldsymbol{\theta},\, \sigma^2\right),
\end{aligned}
$$

$$
\mathcal{X} := \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\} \text{ and } \mathcal{Y} := \{y_1, \ldots, y_N\}
$$

$$p(y_* \mid \boldsymbol{x}_*, \boldsymbol{\theta}^*) = \mathcal{N}\left(y_* \mid \boldsymbol{x}_*^\top \boldsymbol{\theta}^*,\, \sigma^2\right).$$

$$\boldsymbol{\theta}_{\mathrm{ML}} = \arg\max_{\boldsymbol{\theta}} p(\mathcal{Y} \mid \mathcal{X}, \boldsymbol{\theta}).$$

$$-\log p(\mathcal{Y} \mid \mathcal{X}, \boldsymbol{\theta}) = -\log \prod_{n=1}^{N} p(y_n \mid \boldsymbol{x}_n, \boldsymbol{\theta}) = -\sum_{n=1}^{N} \log p(y_n \mid \boldsymbol{x}_n, \boldsymbol{\theta}) \,,$$

$$\log p(y_n \mid \boldsymbol{x}_n, \boldsymbol{\theta}) = -\frac{1}{2\sigma^2}(y_n - \boldsymbol{x}_n^\top \boldsymbol{\theta})^2 + \text{const} \,,$$

$$\mathcal{L}(\boldsymbol{\theta}) := \frac{1}{2\sigma^2}\sum_{n=1}^{N}(y_n - \boldsymbol{x}_n^\top\boldsymbol{\theta})^2$$
$$= \frac{1}{2\sigma^2}(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\theta})^\top(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\theta}) = \frac{1}{2\sigma^2}\|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\theta}\|^2,$$

$$\frac{\mathrm{d}\mathcal{L}}{\mathrm{d}\boldsymbol{\theta}} = \frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\theta}}\left(\frac{1}{2\sigma^2}(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\theta})^\top(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\theta})\right)$$
$$= \frac{1}{2\sigma^2}\frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\theta}}\left(\boldsymbol{y}^\top\boldsymbol{y} - 2\boldsymbol{y}^\top\boldsymbol{X}\boldsymbol{\theta} + \boldsymbol{\theta}^\top\boldsymbol{X}^\top\boldsymbol{X}\boldsymbol{\theta}\right)$$
$$= \frac{1}{\sigma^2}(-\boldsymbol{y}^\top\boldsymbol{X} + \boldsymbol{\theta}^\top\boldsymbol{X}^\top\boldsymbol{X}) \in \mathbb{R}^{1\times D}.$$

$$\frac{\mathrm{d}\mathcal{L}}{\mathrm{d}\boldsymbol{\theta}} = \mathbf{0}^\top \overset{(9.11c)}{\iff} \boldsymbol{\theta}_{\mathrm{ML}}^\top \boldsymbol{X}^\top \boldsymbol{X} = \boldsymbol{y}^\top \boldsymbol{X}$$

$$\iff \boldsymbol{\theta}_{\mathrm{ML}}^\top = \boldsymbol{y}^\top \boldsymbol{X}(\boldsymbol{X}^\top \boldsymbol{X})^{-1}$$

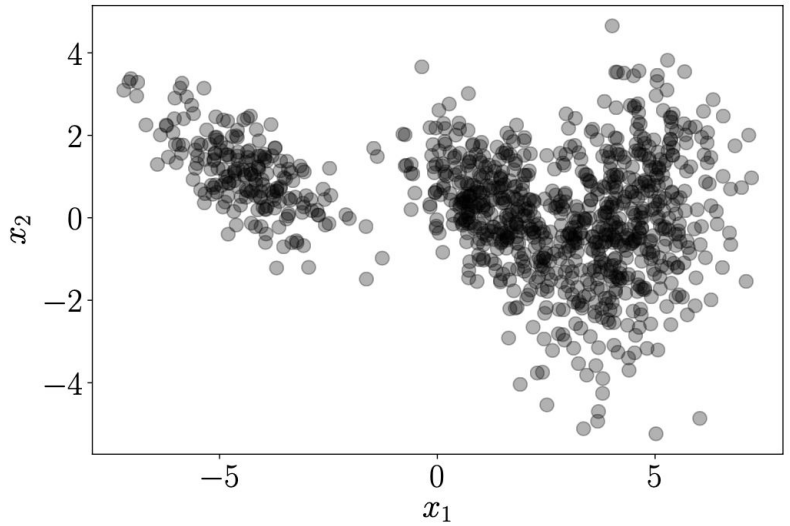
$$\iff \boldsymbol{\theta}_{\mathrm{ML}} = (\boldsymbol{X}^\top \boldsymbol{X})^{-1} \boldsymbol{X}^\top \boldsymbol{y}\,.$$

$$\boldsymbol{\Phi} := \begin{bmatrix} \boldsymbol{\phi}^\top(\boldsymbol{x}_1) \\ \vdots \\ \boldsymbol{\phi}^\top(\boldsymbol{x}_N) \end{bmatrix} = \begin{bmatrix} \phi_0(\boldsymbol{x}_1) & \cdots & \phi_{K-1}(\boldsymbol{x}_1) \\ \phi_0(\boldsymbol{x}_2) & \cdots & \phi_{K-1}(\boldsymbol{x}_2) \\ \vdots & & \vdots \\ \phi_0(\boldsymbol{x}_N) & \cdots & \phi_{K-1}(\boldsymbol{x}_N) \end{bmatrix} \in \mathbb{R}^{N \times K}$$

where $\Phi_{ij} = \phi_j(\boldsymbol{x}_i)$ and $\phi_j : \mathbb{R}^D \to \mathbb{R}$.

$$-\log p(\mathcal{Y} \mid \mathcal{X}, \boldsymbol{\theta}) = \frac{1}{2\sigma^2}(\boldsymbol{y} - \boldsymbol{\Phi}\boldsymbol{\theta})^\top(\boldsymbol{y} - \boldsymbol{\Phi}\boldsymbol{\theta}) + \text{const}\,.$$

$$\boldsymbol{\theta}_{\text{ML}} = (\boldsymbol{\Phi}^\top\boldsymbol{\Phi})^{-1}\boldsymbol{\Phi}^\top\boldsymbol{y}$$

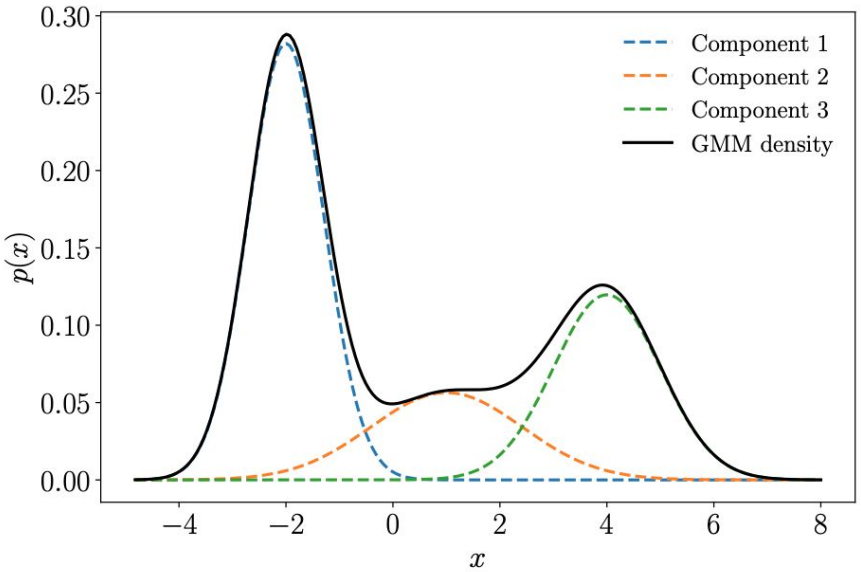

4
2
0
−2
−4
x_2
−5
0
5
x_1

$$p(\boldsymbol{x}) = \sum_{k=1}^{K} \pi_k p_k(\boldsymbol{x})$$

$$0 \leqslant \pi_k \leqslant 1\,, \quad \sum_{k=1}^{K} \pi_k = 1\,,$$

$$p(\boldsymbol{x} \mid \boldsymbol{\theta}) = \sum_{k=1}^{K} \pi_k \mathcal{N}\left(\boldsymbol{x} \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right)$$

$$0 \leqslant \pi_k \leqslant 1\,, \quad \sum_{k=1}^{K} \pi_k = 1\,,$$



$$p(x \mid \boldsymbol{\theta}) = 0.5\mathcal{N}\left(x \mid -2, \tfrac{1}{2}\right) + 0.2\mathcal{N}(x \mid 1, 2) + 0.3\mathcal{N}(x \mid 4, 1)$$

$$p(\mathcal{X} \mid \boldsymbol{\theta}) = \prod_{n=1}^{N} p(\boldsymbol{x}_n \mid \boldsymbol{\theta}), \quad p(\boldsymbol{x}_n \mid \boldsymbol{\theta}) = \sum_{k=1}^{K} \pi_k \mathcal{N}\left(\boldsymbol{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right),$$

$$\log p(\mathcal{X} \mid \boldsymbol{\theta}) = \sum_{n=1}^{N} \log p(\boldsymbol{x}_n \mid \boldsymbol{\theta}) = \underbrace{\sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k \mathcal{N}\left(\boldsymbol{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right)}_{=:\mathcal{L}}.$$

$$\log \mathcal{N}\left(\boldsymbol{x} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma}\right) = -\tfrac{D}{2} \log(2\pi) - \tfrac{1}{2} \log \det(\boldsymbol{\Sigma}) - \tfrac{1}{2} (\boldsymbol{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1} (\boldsymbol{x} - \boldsymbol{\mu}).$$

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{\mu}_k} = \mathbf{0}^\top \iff \sum_{n=1}^{N} \frac{\partial \log p(\boldsymbol{x}_n \mid \boldsymbol{\theta})}{\partial \boldsymbol{\mu}_k} = \mathbf{0}^\top,$$

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{\Sigma}_k} = \mathbf{0} \iff \sum_{n=1}^{N} \frac{\partial \log p(\boldsymbol{x}_n \mid \boldsymbol{\theta})}{\partial \boldsymbol{\Sigma}_k} = \mathbf{0},$$

$$\frac{\partial \mathcal{L}}{\partial \pi_k} = 0 \iff \sum_{n=1}^{N} \frac{\partial \log p(\boldsymbol{x}_n \mid \boldsymbol{\theta})}{\partial \pi_k} = 0.$$

$$\frac{\partial \log p(\boldsymbol{x}_n \mid \boldsymbol{\theta})}{\partial \boldsymbol{\theta}} = \frac{1}{p(\boldsymbol{x}_n \mid \boldsymbol{\theta})} \frac{\partial p(\boldsymbol{x}_n \mid \boldsymbol{\theta})}{\partial \boldsymbol{\theta}},$$

$$\frac{1}{p(\boldsymbol{x}_n \mid \boldsymbol{\theta})} = \frac{1}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\boldsymbol{x}_n \mid \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}.$$

$$r_{nk} := \frac{\pi_k \mathcal{N}\left(\boldsymbol{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right)}{\sum_{j=1}^{K} \pi_j \mathcal{N}\left(\boldsymbol{x}_n \mid \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j\right)}$$

$$p\left(\boldsymbol{x}_n \mid \pi_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right) = \pi_k \mathcal{N}\left(\boldsymbol{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right)$$

$$\boldsymbol{r}_n := \left[r_{n1}, \ldots, r_{nK}\right]^\top$$

$$\boldsymbol{\mu}_k^{new} = \frac{\sum_{n=1}^{N} r_{nk}\boldsymbol{x}_n}{\sum_{n=1}^{N} r_{nk}} ,$$

$$\boldsymbol{\Sigma}_k^{new} = \frac{1}{N_k}\sum_{n=1}^{N} r_{nk}(\boldsymbol{x}_n - \boldsymbol{\mu}_k)(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^\top ,$$

$$\pi_k^{new} = \frac{N_k}{N} , \quad k = 1, \ldots, K ,$$

$$\boldsymbol{\mu}_k^{new} = \frac{\sum_{n=1}^{N} r_{nk} \boldsymbol{x}_n}{\sum_{n=1}^{N} r_{nk}},$$

$$\frac{\partial p(\boldsymbol{x}_n \mid \boldsymbol{\theta})}{\partial \boldsymbol{\mu}_k} = \sum_{j=1}^{K} \pi_j \frac{\partial \mathcal{N}\left(\boldsymbol{x}_n \mid \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j\right)}{\partial \boldsymbol{\mu}_k} = \pi_k \frac{\partial \mathcal{N}\left(\boldsymbol{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right)}{\partial \boldsymbol{\mu}_k}$$

$$= \pi_k (\boldsymbol{x}_n - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1} \mathcal{N}\left(\boldsymbol{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right),$$

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{\mu}_k} = \sum_{n=1}^{N} \frac{\partial \log p(\boldsymbol{x}_n \mid \boldsymbol{\theta})}{\partial \boldsymbol{\mu}_k} = \sum_{n=1}^{N} \frac{1}{p(\boldsymbol{x}_n \mid \boldsymbol{\theta})} \frac{\partial p(\boldsymbol{x}_n \mid \boldsymbol{\theta})}{\partial \boldsymbol{\mu}_k}$$

$$= \sum_{n=1}^{N} (\boldsymbol{x}_n - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1} \underbrace{\frac{\pi_k \mathcal{N}(\boldsymbol{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\boldsymbol{x}_n \mid \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}}_{=r_{nk}}$$

$$= \sum_{n=1}^{N} r_{nk} (\boldsymbol{x}_n - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1} .$$

$$\sum_{n=1}^{N} r_{nk}\boldsymbol{x}_n = \sum_{n=1}^{N} r_{nk}\boldsymbol{\mu}_k^{\text{new}} \iff \boldsymbol{\mu}_k^{\text{new}} = \frac{\sum_{n=1}^{N} r_{nk}\boldsymbol{x}_n}{\boxed{\sum_{n=1}^{N} r_{nk}}} = \frac{1}{\boxed{N_k}} \sum_{n=1}^{N} r_{nk}\boldsymbol{x}_n \,,$$

$$N_k := \sum_{n=1}^{N} r_{nk}$$

$$\boldsymbol{\Sigma}_k^{new} = \frac{1}{N_k} \sum_{n=1}^{N} r_{nk} (\boldsymbol{x}_n - \boldsymbol{\mu}_k)(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^\top ,$$

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{\Sigma}_k} = \sum_{n=1}^{N} \frac{\partial \log p(\boldsymbol{x}_n \mid \boldsymbol{\theta})}{\partial \boldsymbol{\Sigma}_k} = \sum_{n=1}^{N} \frac{1}{p(\boldsymbol{x}_n \mid \boldsymbol{\theta})} \frac{\partial p(\boldsymbol{x}_n \mid \boldsymbol{\theta})}{\partial \boldsymbol{\Sigma}_k} .$$

$$\frac{\partial p(\boldsymbol{x}_n \mid \boldsymbol{\theta})}{\partial \boldsymbol{\Sigma}_k} \tag{11.32a}$$

$$= \frac{\partial}{\partial \boldsymbol{\Sigma}_k} \left(\pi_k (2\pi)^{-\frac{D}{2}} \det(\boldsymbol{\Sigma}_k)^{-\frac{1}{2}} \exp\left(-\tfrac{1}{2}(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1}(\boldsymbol{x}_n - \boldsymbol{\mu}_k)\right) \right) \tag{11.32b}$$

$$= \pi_k (2\pi)^{-\frac{D}{2}} \left[\frac{\partial}{\partial \boldsymbol{\Sigma}_k} \det(\boldsymbol{\Sigma}_k)^{-\frac{1}{2}} \exp\left(-\tfrac{1}{2}(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1}(\boldsymbol{x}_n - \boldsymbol{\mu}_k)\right) \right.$$

$$\left. + \det(\boldsymbol{\Sigma}_k)^{-\frac{1}{2}} \frac{\partial}{\partial \boldsymbol{\Sigma}_k} \exp\left(-\tfrac{1}{2}(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1}(\boldsymbol{x}_n - \boldsymbol{\mu}_k)\right) \right] . \tag{11.32c}$$

$$\frac{\partial}{\partial \boldsymbol{\Sigma}_k} \det(\boldsymbol{\Sigma}_k)^{-\frac{1}{2}} \overset{(5.101)}{=} -\frac{1}{2} \det(\boldsymbol{\Sigma}_k)^{-\frac{1}{2}} \boldsymbol{\Sigma}_k^{-1}, \tag{11.33}$$

$$\frac{\partial}{\partial \boldsymbol{\Sigma}_k} (\boldsymbol{x}_n - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1} (\boldsymbol{x}_n - \boldsymbol{\mu}_k) \overset{(5.106)}{=} -\boldsymbol{\Sigma}_k^{-1} (\boldsymbol{x}_n - \boldsymbol{\mu}_k)(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1} \tag{11.34}$$

$$\frac{\partial p(\boldsymbol{x}_n \mid \boldsymbol{\theta})}{\partial \boldsymbol{\Sigma}_k} = \pi_k \mathcal{N}\left(\boldsymbol{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right) \cdot \left[-\tfrac{1}{2}(\boldsymbol{\Sigma}_k^{-1} - \boldsymbol{\Sigma}_k^{-1}(\boldsymbol{x}_n - \boldsymbol{\mu}_k)(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1})\right].$$

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{\Sigma}_k} = \sum_{n=1}^{N} \frac{\partial \log p(\boldsymbol{x}_n \mid \boldsymbol{\theta})}{\partial \boldsymbol{\Sigma}_k} = \sum_{n=1}^{N} \frac{1}{p(\boldsymbol{x}_n \mid \boldsymbol{\theta})} \frac{\partial p(\boldsymbol{x}_n \mid \boldsymbol{\theta})}{\partial \boldsymbol{\Sigma}_k}$$

$$= \sum_{n=1}^{N} \underbrace{\frac{\pi_k \mathcal{N}(\boldsymbol{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\boldsymbol{x}_n \mid \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}}_{=r_{nk}}$$

$$\cdot \left[-\tfrac{1}{2} (\boldsymbol{\Sigma}_k^{-1} - \boldsymbol{\Sigma}_k^{-1} (\boldsymbol{x}_n - \boldsymbol{\mu}_k)(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1}) \right]$$

$$= -\frac{1}{2}\sum_{n=1}^{N} r_{nk}(\boldsymbol{\Sigma}_k^{-1} - \boldsymbol{\Sigma}_k^{-1}(\boldsymbol{x}_n - \boldsymbol{\mu}_k)(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1}) \qquad (11.36c)$$

$$= -\frac{1}{2}\boldsymbol{\Sigma}_k^{-1}\underbrace{\sum_{n=1}^{N} r_{nk}}_{=N_k} + \frac{1}{2}\boldsymbol{\Sigma}_k^{-1}\left(\sum_{n=1}^{N} r_{nk}(\boldsymbol{x}_n - \boldsymbol{\mu}_k)(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^\top\right)\boldsymbol{\Sigma}_k^{-1}.$$

$$N_k \boldsymbol{\Sigma}_k^{-1} = \boldsymbol{\Sigma}_k^{-1} \left(\sum_{n=1}^{N} r_{nk} (\boldsymbol{x}_n - \boldsymbol{\mu}_k)(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^\top \right) \boldsymbol{\Sigma}_k^{-1}$$

$$\iff N_k \boldsymbol{I} = \left(\sum_{n=1}^{N} r_{nk} (\boldsymbol{x}_n - \boldsymbol{\mu}_k)(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^\top \right) \boldsymbol{\Sigma}_k^{-1} .$$

$$\boldsymbol{\Sigma}_k^{\text{new}} = \frac{1}{N_k} \sum_{n=1}^{N} r_{nk} (\boldsymbol{x}_n - \boldsymbol{\mu}_k)(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^\top ,$$

$$\pi_k^{new} = \frac{N_k}{N}, \quad k = 1, \ldots, K,$$

$$\mathfrak{L} = \mathcal{L} + \lambda \left(\sum_{k=1}^{K} \pi_k - 1 \right)$$

$$= \sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k \mathcal{N}\left(\boldsymbol{x}_n \,|\, \boldsymbol{\mu}_k,\, \boldsymbol{\Sigma}_k\right) + \lambda \left(\sum_{k=1}^{K} \pi_k - 1 \right) ,$$

$$\frac{\partial \mathfrak{L}}{\partial \pi_k} = \sum_{n=1}^{N} \frac{\mathcal{N}\left(\boldsymbol{x}_n \,|\, \boldsymbol{\mu}_k,\, \boldsymbol{\Sigma}_k\right)}{\sum_{j=1}^{K} \pi_j \mathcal{N}\left(\boldsymbol{x}_n \,|\, \boldsymbol{\mu}_j,\, \boldsymbol{\Sigma}_j\right)} + \lambda$$

$$= \frac{1}{\pi_k} \underbrace{\sum_{n=1}^{N} \frac{\pi_k \mathcal{N}\left(\boldsymbol{x}_n \,|\, \boldsymbol{\mu}_k,\, \boldsymbol{\Sigma}_k\right)}{\sum_{j=1}^{K} \pi_j \mathcal{N}\left(\boldsymbol{x}_n \,|\, \boldsymbol{\mu}_j,\, \boldsymbol{\Sigma}_j\right)}}_{=N_k} + \lambda = \frac{N_k}{\pi_k} + \lambda \,,$$

$$\frac{\partial \mathfrak{L}}{\partial \lambda} = \sum_{k=1}^{K} \pi_k - 1 \,.$$

$$\pi_k = -\frac{N_k}{\lambda}\,,$$

$$1 = \sum_{k=1}^{K} \pi_k\,.$$

$$\sum_{k=1}^{K} \pi_k = 1 \iff -\sum_{k=1}^{K} \frac{N_k}{\lambda} = 1 \iff -\frac{N}{\lambda} = 1 \iff \lambda = -N\,.$$

1. Initialize $\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k, \pi_k$.
2. *E-step:* Evaluate responsibilities r_{nk} for every data point $\boldsymbol{x}_n$ using current parameters $\pi_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k$:

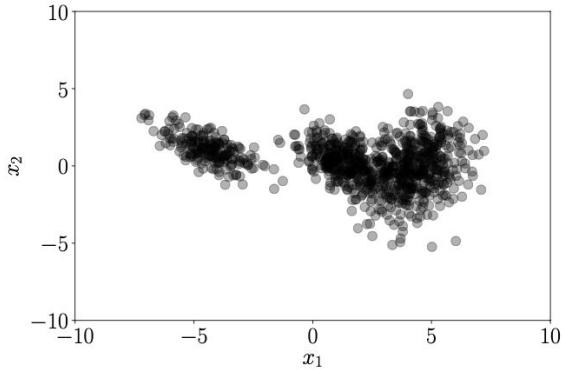
$$r_{nk} = \frac{\pi_k \mathcal{N}\left(\boldsymbol{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right)}{\sum_j \pi_j \mathcal{N}\left(\boldsymbol{x}_n \mid \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j\right)} . \tag{11.53}$$

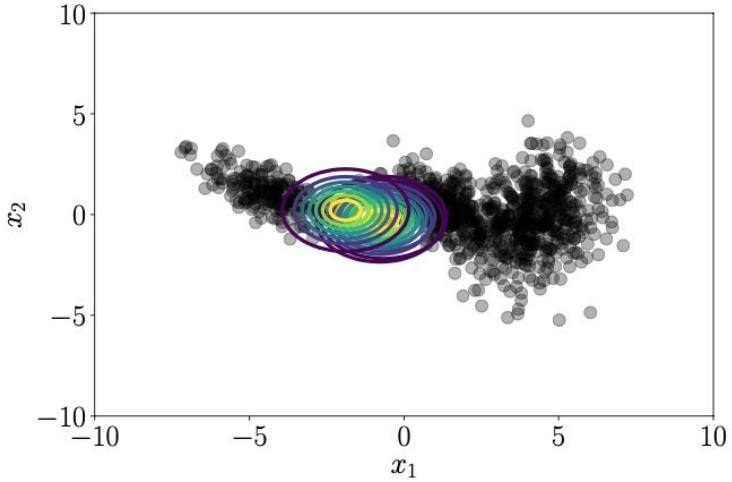
3. *M-step:* Reestimate parameters $\pi_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k$ using the current responsibilities r_{nk} (from E-step):

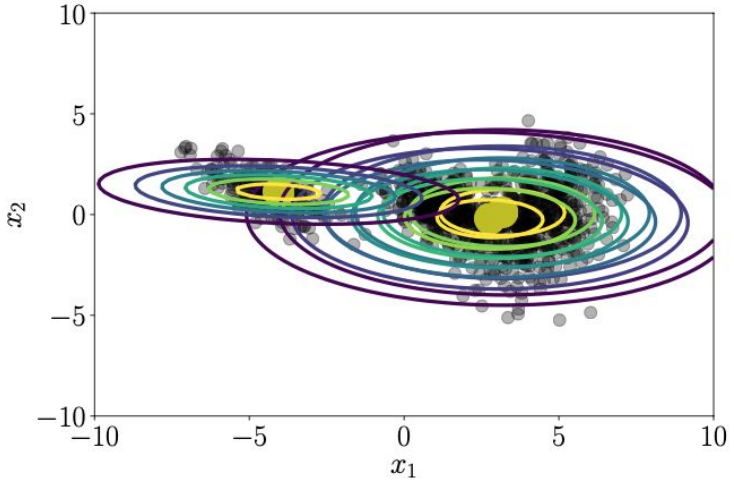
$$\boldsymbol{\mu}_k = \frac{1}{N_k} \sum_{n=1}^{N} r_{nk} \boldsymbol{x}_n , \tag{11.54}$$

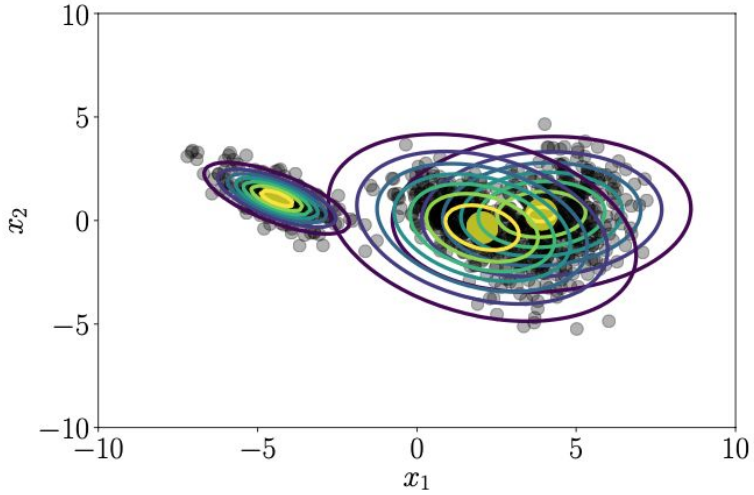
$$\boldsymbol{\Sigma}_k = \frac{1}{N_k} \sum_{n=1}^{N} r_{nk} (\boldsymbol{x}_n - \boldsymbol{\mu}_k)(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^\top , \tag{11.55}$$

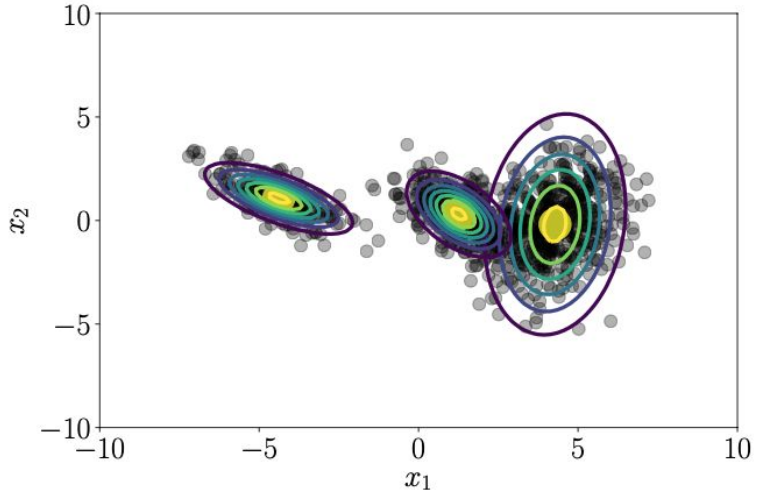
$$\pi_k = \frac{N_k}{N} . \tag{11.56}$$

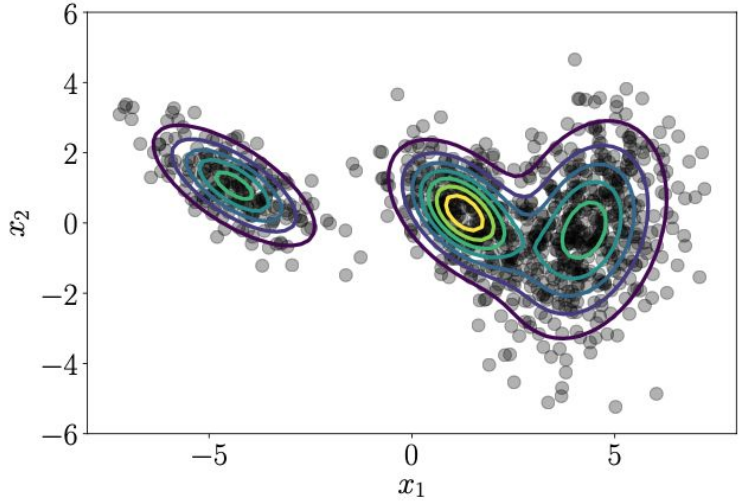

10
5
0
−5
−10
−10
−5
0
5
10
x_2
x_1

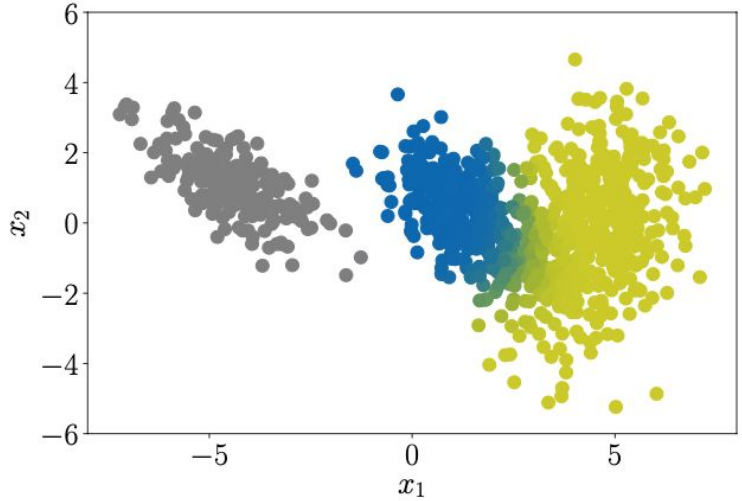

10
5
0
−5
−10
x_2
−10
−5
0
5
10
x_1


10
5
0
−5
−10
x_2
−10
−5
0
5
10
x_1

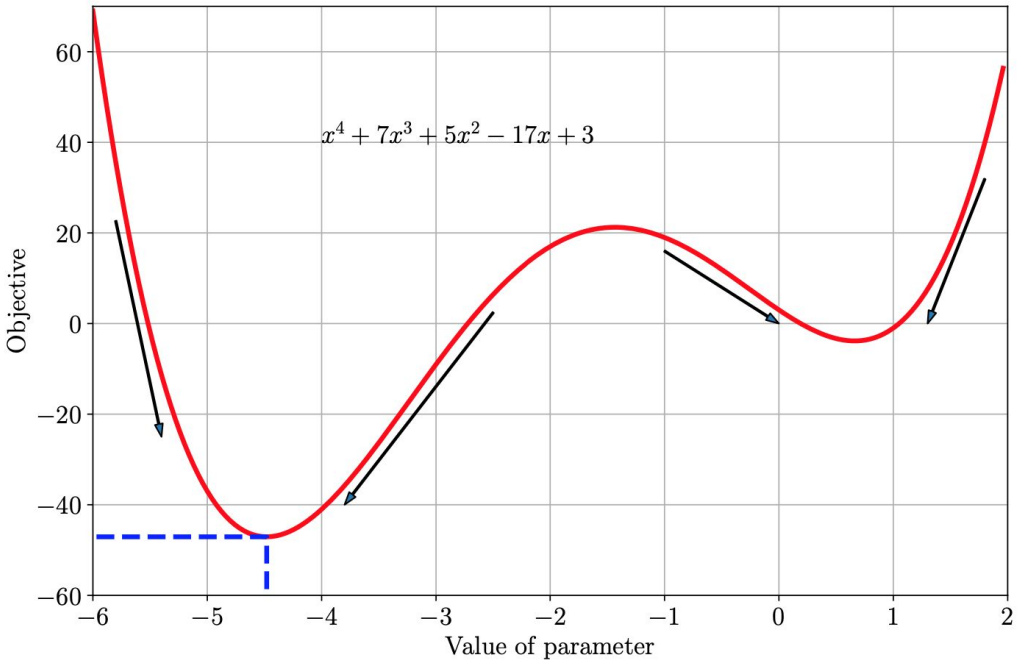

10
5
0
−5
−10
x_2
−10
−5
0
5
10
x_1


10
5
0
−5
−10
x_2
−10
−5
0
5
10
x_1


6
4
2
0
−2
−4
−6
−5
0
5
x_1
x_2


6
4
2
0
−2
−4
−6
−5
0
5
x_1
x_2

Optimization for Machine learning


$x^4 + 7x^3 + 5x^2 - 17x + 3$
Objective
Value of parameter
60
40
20
0
−20
−40
−60
−6
−5
−4
−3
−2
−1
0
1
2

$$\min_{\boldsymbol{x}} f(\boldsymbol{x}) \,,$$

$$f \,:\, \mathbb{R}^d \,\rightarrow\, \mathbb{R}$$

$$\boldsymbol{x}_1 = \boldsymbol{x}_0 - \gamma((\nabla f)(\boldsymbol{x}_0))^\top$$

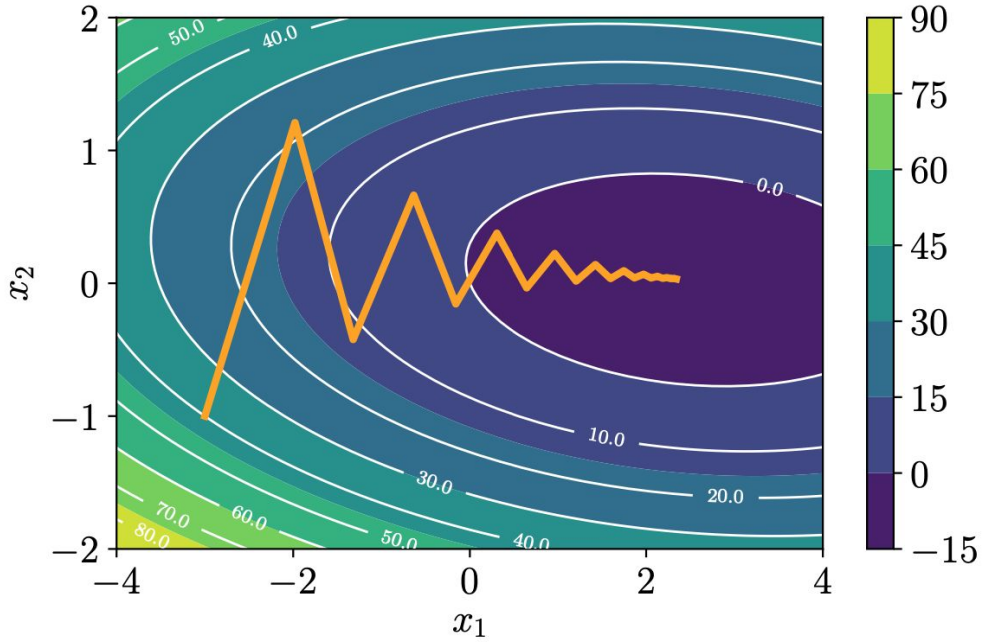
for a small *step-size* $\gamma \geqslant 0$, then $f(\boldsymbol{x}_1) \leqslant f(\boldsymbol{x}_0)$

$$\boldsymbol{x}_{i+1} = \boldsymbol{x}_i - \gamma_i((\nabla f)(\boldsymbol{x}_i))^\top .$$

$$f\left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}\right) = \frac{1}{2} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^\top \begin{bmatrix} 2 & 1 \\ 1 & 20 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} - \begin{bmatrix} 5 \\ 3 \end{bmatrix}^\top \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

$$\nabla f\left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}\right) = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^\top \begin{bmatrix} 2 & 1 \\ 1 & 20 \end{bmatrix} - \begin{bmatrix} 5 \\ 3 \end{bmatrix}^\top .$$

$$\boldsymbol{x}_0 = [-3, -1]^\top \qquad \gamma = 0.085$$


2
1
0
−1
−2
−4
−2
0
2
4
x_1
x_2
50.0
40.0
0.0
10.0
30.0
20.0
70.0
60.0
50.0
40.0
80.0
90
75
60
45
30
15
0
−15

- When the function value increases after a gradient step, the step-size was too large. Undo the step and decrease the step-size.
- When the function value decreases the step could have been larger. Try to increase the step-size.

$$\boldsymbol{x}_{i+1} = \boldsymbol{x}_i - \gamma_i((\nabla f)(\boldsymbol{x}_i))^\top + \alpha\Delta\boldsymbol{x}_i$$
$$\Delta\boldsymbol{x}_i = \boldsymbol{x}_i - \boldsymbol{x}_{i-1} = \alpha\Delta\boldsymbol{x}_{i-1} - \gamma_{i-1}((\nabla f)(\boldsymbol{x}_{i-1}))^\top,$$

$$\alpha \in [0, 1]$$

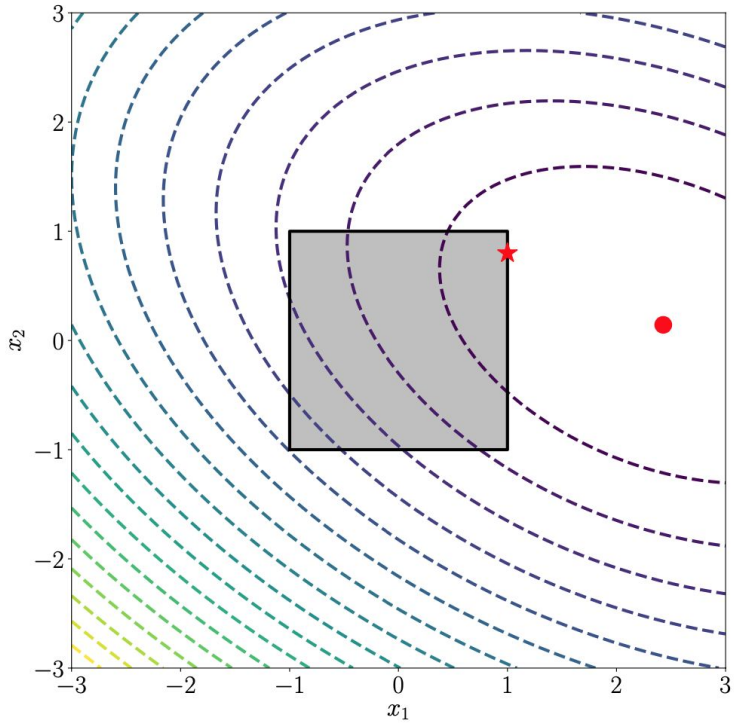
stochastic gradient descent (often shortened as SGD) is a stochastic approximation of the gradient descent method for minimizing an objective function that is written as a sum of differentiable functions.

$$L(\boldsymbol{\theta}) = \sum_{n=1}^{N} L_n(\boldsymbol{\theta}) \,,$$

$$L(\boldsymbol{\theta}) = -\sum_{n=1}^{N} \log p(y_n | \boldsymbol{x}_n, \boldsymbol{\theta}) \,,$$

$$\boldsymbol{\theta}_{i+1} = \boldsymbol{\theta}_i - \gamma_i (\nabla L(\boldsymbol{\theta}_i))^\top = \boldsymbol{\theta}_i - \gamma_i \sum_{n=1}^{N} (\nabla L_n(\boldsymbol{\theta}_i))^\top$$

$$\begin{aligned} \min_{\boldsymbol{x}} \quad & f(\boldsymbol{x}) \\ \text{subject to} \quad & g_i(\boldsymbol{x}) \leqslant 0 \quad \text{for all} \quad i = 1, \ldots, m\,. \end{aligned}$$


3
2
1
0
−1
−2
−3
x_2
−3
−2
−1
0
1
2
3
x_1

$$J(\boldsymbol{x}) = f(\boldsymbol{x}) + \sum_{i=1}^{m} \mathbf{1}(g_i(\boldsymbol{x}))\,,$$

$$\mathbf{1}(z) = \begin{cases} 0 & \text{if } z \leqslant 0 \\ \infty & \text{otherwise} \end{cases}.$$

$$\begin{aligned}\mathfrak{L}(\boldsymbol{x}, \boldsymbol{\lambda}) &= f(\boldsymbol{x}) + \sum_{i=1}^{m} \lambda_i g_i(\boldsymbol{x}) \\ &= f(\boldsymbol{x}) + \boldsymbol{\lambda}^\top \boldsymbol{g}(\boldsymbol{x}) \,,\end{aligned}$$

$$\begin{aligned} \min_{\boldsymbol{x}} \quad & f(\boldsymbol{x}) \\ \text{subject to} \quad & g_i(\boldsymbol{x}) \leqslant 0 \quad \text{for all} \quad i = 1, \ldots, m \end{aligned}$$

$$\begin{aligned} \max_{\boldsymbol{\lambda} \in \mathbb{R}^m} \quad & \mathfrak{D}(\boldsymbol{\lambda}) \\ \text{subject to} \quad & \boldsymbol{\lambda} \geqslant \mathbf{0}, \end{aligned}$$

where $\boldsymbol{\lambda}$ are the dual variables and $\mathfrak{D}(\boldsymbol{\lambda}) = \min_{\boldsymbol{x} \in \mathbb{R}^d} \mathfrak{L}(\boldsymbol{x}, \boldsymbol{\lambda})$.

$$\max_{\boldsymbol{y}} \min_{\boldsymbol{x}} \varphi(\boldsymbol{x}, \boldsymbol{y}) \leqslant \min_{\boldsymbol{x}} \max_{\boldsymbol{y}} \varphi(\boldsymbol{x}, \boldsymbol{y}) \,.$$

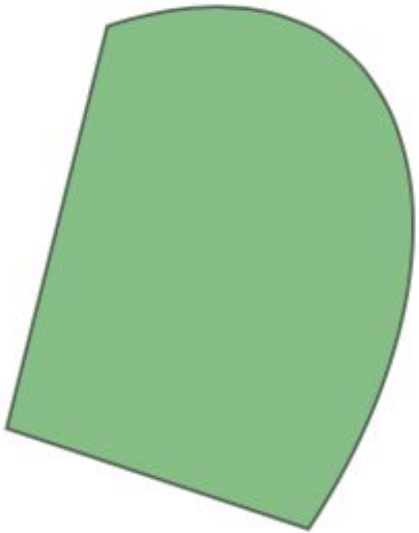
For all $\boldsymbol{x}, \boldsymbol{y}$ $\qquad$ $\min_{\boldsymbol{x}} \varphi(\boldsymbol{x}, \boldsymbol{y}) \leqslant \max_{\boldsymbol{y}} \varphi(\boldsymbol{x}, \boldsymbol{y}) \,.$

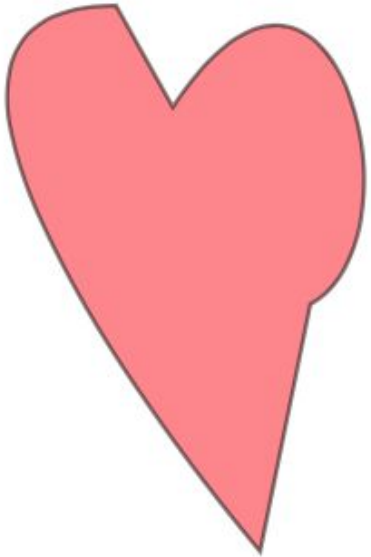
$$J(\boldsymbol{x}) = \max_{\boldsymbol{\lambda} \geqslant \mathbf{0}} \mathfrak{L}(\boldsymbol{x}, \boldsymbol{\lambda}) \, .$$

$$\min_{\boldsymbol{x} \in \mathbb{R}^d} \max_{\boldsymbol{\lambda} \geqslant \mathbf{0}} \mathfrak{L}(\boldsymbol{x}, \boldsymbol{\lambda}) \, .$$

$$\min_{\boldsymbol{x}\in\mathbb{R}^d}\max_{\boldsymbol{\lambda}\geqslant\mathbf{0}}\mathfrak{L}(\boldsymbol{x},\boldsymbol{\lambda})\geqslant\max_{\boldsymbol{\lambda}\geqslant\mathbf{0}}\min_{\boldsymbol{x}\in\mathbb{R}^d}\mathfrak{L}(\boldsymbol{x},\boldsymbol{\lambda})\,.$$

$$
\begin{aligned}
\min_{\boldsymbol{x}} \quad & f(\boldsymbol{x}) \\
\text{subject to} \quad & g_i(\boldsymbol{x}) \leqslant 0 \quad \text{for all} \quad i = 1, \ldots, m \\
& h_j(\boldsymbol{x}) = 0 \quad \text{for all} \quad j = 1, \ldots, n\,.
\end{aligned}
$$





Definition 7.2. A set $\mathcal{C}$ is a *convex set* if for any $x, y \in \mathcal{C}$ and for any scalar θ with $0 \leqslant \theta \leqslant 1$, we have

$$\theta x + (1 - \theta) y \in \mathcal{C} \,. \tag{7.29}$$

Definition 7.3. Let function $f : \mathbb{R}^D \to \mathbb{R}$ be a function whose domain is a convex set. The function f is a *convex function* if for all $\boldsymbol{x}, \boldsymbol{y}$ in the domain of f, and for any scalar θ with $0 \leqslant \theta \leqslant 1$, we have

$$f(\theta \boldsymbol{x} + (1 - \theta) \boldsymbol{y}) \leqslant \theta f(\boldsymbol{x}) + (1 - \theta) f(\boldsymbol{y}) \,. \tag{7.30}$$

$$f(\boldsymbol{y}) \geqslant f(\boldsymbol{x}) + \nabla_{\boldsymbol{x}} f(\boldsymbol{x})^{\top} (\boldsymbol{y} - \boldsymbol{x}) \,.$$

$$\begin{aligned} \min_{\boldsymbol{x} \in \mathbb{R}^d} \quad & \boldsymbol{c}^\top \boldsymbol{x} \\ \text{subject to} \quad & \boldsymbol{A}\boldsymbol{x} \leqslant \boldsymbol{b}\,, \end{aligned}$$

$$\mathfrak{L}(\boldsymbol{x}, \boldsymbol{\lambda}) = \boldsymbol{c}^\top \boldsymbol{x} + \boldsymbol{\lambda}^\top (\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b}) \,,$$

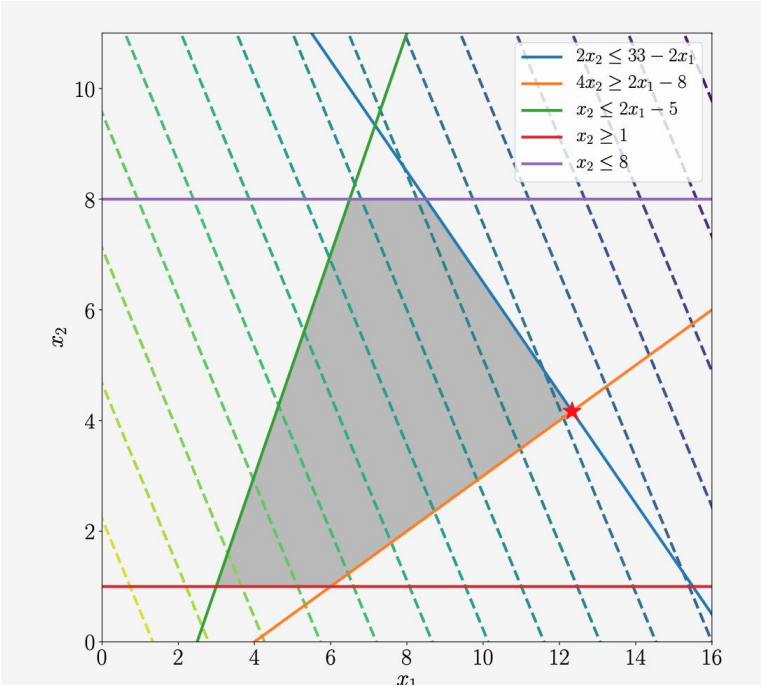
$$\mathfrak{L}(\boldsymbol{x}, \boldsymbol{\lambda}) = (\boldsymbol{c} + \boldsymbol{A}^\top \boldsymbol{\lambda})^\top \boldsymbol{x} - \boldsymbol{\lambda}^\top \boldsymbol{b} \,.$$

$$\mathfrak{D}(\boldsymbol{\lambda}) = -\boldsymbol{\lambda}^\top \boldsymbol{b}.$$

$$\begin{aligned} \max_{\boldsymbol{\lambda} \in \mathbb{R}^m} \quad & -\boldsymbol{b}^\top \boldsymbol{\lambda} \\ \text{subject to} \quad & \boldsymbol{c} + \boldsymbol{A}^\top \boldsymbol{\lambda} = \boldsymbol{0} \\ & \boldsymbol{\lambda} \geqslant \boldsymbol{0}. \end{aligned}$$

$$\min_{\boldsymbol{x}\in\mathbb{R}^2} \quad -\begin{bmatrix}5\\3\end{bmatrix}^\top \begin{bmatrix}x_1\\x_2\end{bmatrix}$$

$$\text{subject to} \quad \begin{bmatrix}2 & 2\\2 & -4\\-2 & 1\\0 & -1\\0 & 1\end{bmatrix} \begin{bmatrix}x_1\\x_2\end{bmatrix} \leqslant \begin{bmatrix}33\\8\\5\\-1\\8\end{bmatrix}$$


$2x_2 \leq 33 - 2x_1$
$4x_2 \geq 2x_1 - 8$
$x_2 \leq 2x_1 - 5$
$x_2 \geq 1$
$x_2 \leq 8$
x_2
x_1
0
2
4
6
8
10
12
14
16

$$\begin{aligned} \min_{\boldsymbol{x} \in \mathbb{R}^d} \quad & \frac{1}{2} \boldsymbol{x}^\top \boldsymbol{Q} \boldsymbol{x} + \boldsymbol{c}^\top \boldsymbol{x} \\ \text{subject to} \quad & \boldsymbol{A} \boldsymbol{x} \leqslant \boldsymbol{b}\,, \end{aligned}$$

$$\begin{aligned}\mathfrak{L}(\boldsymbol{x}, \boldsymbol{\lambda}) &= \frac{1}{2}\boldsymbol{x}^\top \boldsymbol{Q}\boldsymbol{x} + \boldsymbol{c}^\top \boldsymbol{x} + \boldsymbol{\lambda}^\top (\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b}) \\ &= \frac{1}{2}\boldsymbol{x}^\top \boldsymbol{Q}\boldsymbol{x} + (\boldsymbol{c} + \boldsymbol{A}^\top \boldsymbol{\lambda})^\top \boldsymbol{x} - \boldsymbol{\lambda}^\top \boldsymbol{b}\,,\end{aligned}$$

$$\boldsymbol{Q}\boldsymbol{x} + (\boldsymbol{c} + \boldsymbol{A}^\top \boldsymbol{\lambda}) = \boldsymbol{0}\,.$$

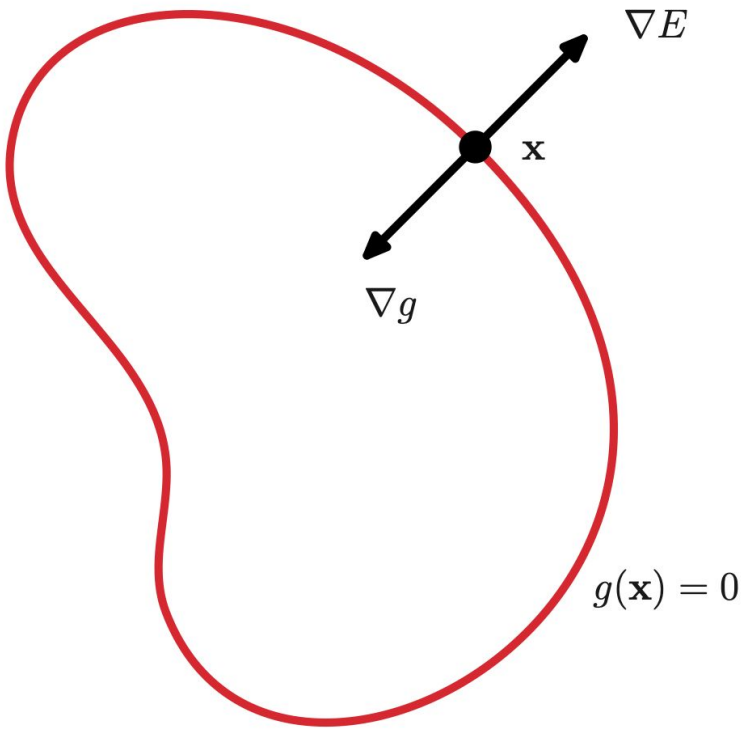
$$\boldsymbol{x} = -\boldsymbol{Q}^{-1}(\boldsymbol{c} + \boldsymbol{A}^\top \boldsymbol{\lambda})\,.$$

$$\mathfrak{D}(\boldsymbol{\lambda}) = -\frac{1}{2}(\boldsymbol{c} + \boldsymbol{A}^\top \boldsymbol{\lambda})^\top \boldsymbol{Q}^{-1}(\boldsymbol{c} + \boldsymbol{A}^\top \boldsymbol{\lambda}) - \boldsymbol{\lambda}^\top \boldsymbol{b}\,.$$

$$\begin{aligned} \max_{\boldsymbol{\lambda} \in \mathbb{R}^m} \quad & -\frac{1}{2}(\boldsymbol{c} + \boldsymbol{A}^\top \boldsymbol{\lambda})^\top \boldsymbol{Q}^{-1}(\boldsymbol{c} + \boldsymbol{A}^\top \boldsymbol{\lambda}) - \boldsymbol{\lambda}^\top \boldsymbol{b} \\ \text{subject to} \quad & \boldsymbol{\lambda} \geqslant \boldsymbol{0}\,. \end{aligned}$$

$$E(\mathbf{x}) = E(x_1, x_2, ...x_D)$$

$$g(\mathbf{x}) = 0$$



$$E(\mathbf{x}) = E(x_1, x_2, ...x_D) \qquad \nabla E = 0$$

$$g(\mathbf{x}) = 0 \qquad \nabla E + \lambda \nabla g = 0$$

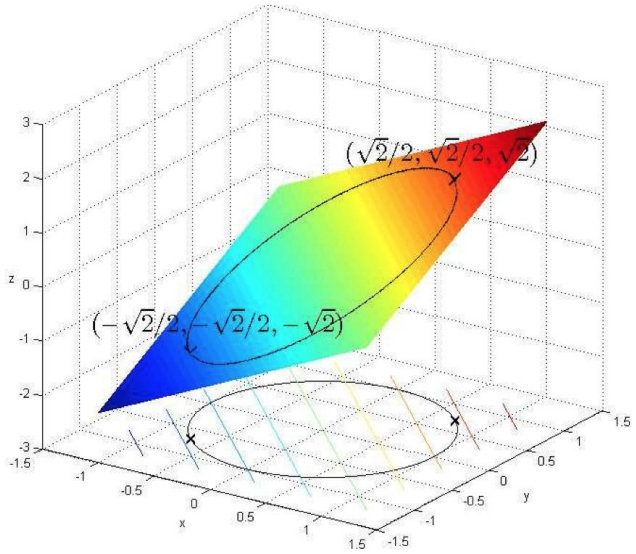
$$L(\mathbf{x}, \lambda) = E(\mathbf{x}) + \lambda g(\mathbf{x})$$

$$\frac{dL}{d\lambda} = g(\mathbf{x}) = 0$$

$$\frac{dL}{d\mathbf{x}} = \nabla E + \lambda \nabla g = 0$$

$$\arg\min_{x,y} x + y$$

$$\text{subject to } x^2 + y^2 = 1$$

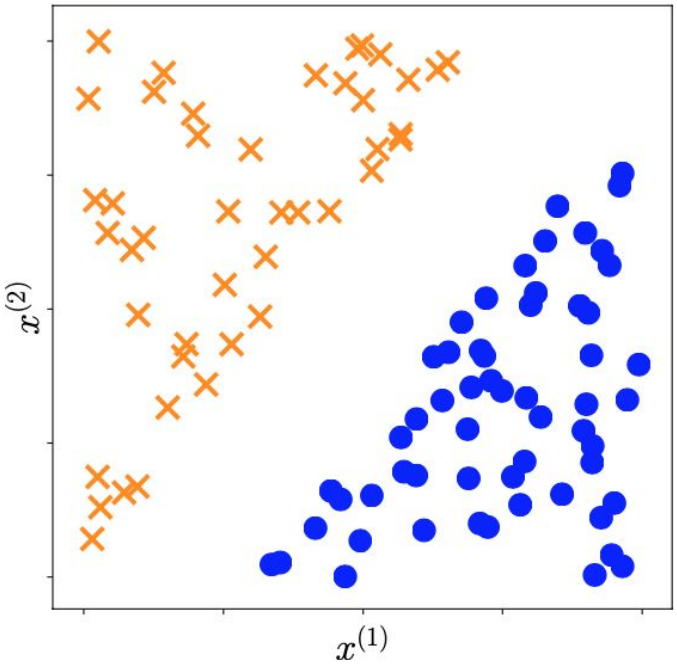


$$L(x, y, \lambda) = x + y + \lambda(x^2 + y^2 - 1)$$

$$\begin{aligned}
\frac{dL}{dx} &= 1 + 2\lambda x = 0 \\
\frac{dL}{dy} &= 1 + 2\lambda y = 0 \\
\frac{dL}{d\lambda} &= x^2 + y^2 - 1 = 0
\end{aligned}$$

$$x = y = \pm\frac{1}{\sqrt{2}}.$$

$$x = y = -\frac{1}{\sqrt{2}}$$


$x^{(2)}$
$x^{(1)}$

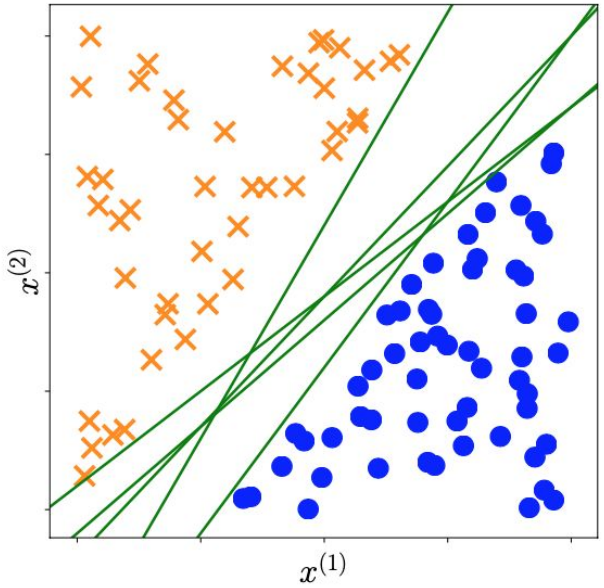
$$f : \mathbb{R}^D \to \mathbb{R}$$
$$\boldsymbol{x} \mapsto \langle \boldsymbol{w}, \boldsymbol{x} \rangle + b \,,$$

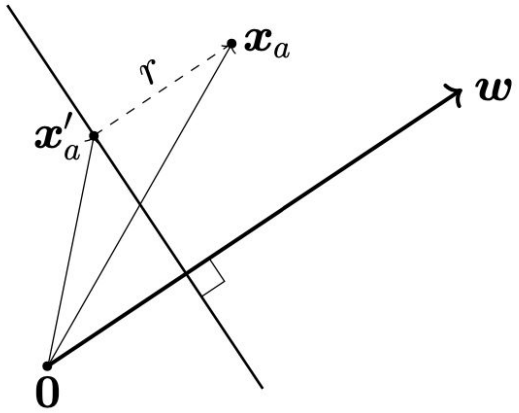
$$\left\{ \boldsymbol{x} \in \mathbb{R}^D : f(\boldsymbol{x}) = 0 \right\} \,.$$

$$\langle \boldsymbol{w}, \boldsymbol{x}_n \rangle + b \geqslant 0 \quad \text{when} \quad y_n = +1$$

$$\langle \boldsymbol{w}, \boldsymbol{x}_n \rangle + b < 0 \quad \text{when} \quad y_n = -1\,.$$

$$y_n(\langle \boldsymbol{w}, \boldsymbol{x}_n \rangle + b) \geqslant 0\,.$$

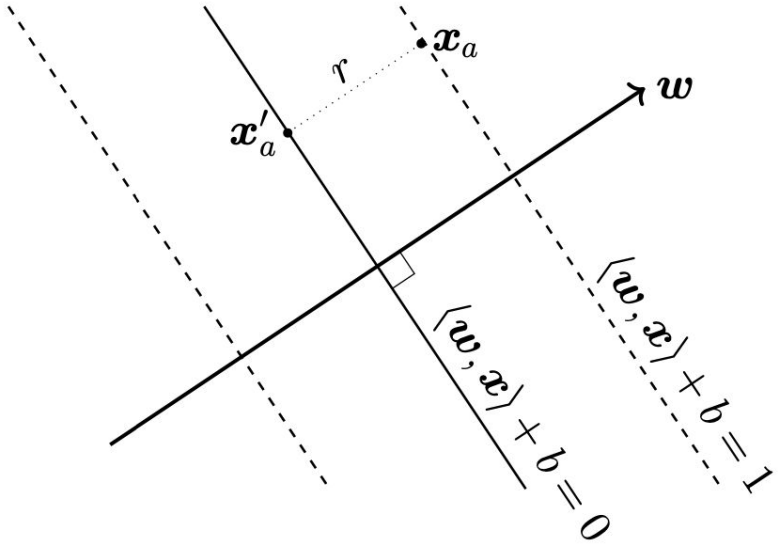

$x^{(2)}$
$x^{(1)}$



$$\boldsymbol{x}_a = \boldsymbol{x}'_a + r\frac{\boldsymbol{w}}{\|\boldsymbol{w}\|}\,.$$

$$y_n(\langle \boldsymbol{w}, \boldsymbol{x}_n \rangle + b) \geqslant r \,.$$

$$\|\boldsymbol{w}\| = 1,$$


x_a
r
x'_a
w
$\langle w, x \rangle + b = 1$
$\langle w, x \rangle + b = 0$

$$\max_{\boldsymbol{w},b,r} \quad \underbrace{r}_{\text{margin}}$$

$$\text{subject to} \quad \underbrace{y_n(\langle \boldsymbol{w}, \boldsymbol{x}_n \rangle + b) \geqslant r}_{\text{data fitting}}, \underbrace{\|\boldsymbol{w}\| = 1}_{\text{normalization}}, \quad r > 0,$$

$$\langle \boldsymbol{w}, \boldsymbol{x}'_a \rangle + b = 0\,.$$

$$\left\langle \boldsymbol{w}, \boldsymbol{x}_a - r\frac{\boldsymbol{w}}{\|\boldsymbol{w}\|} \right\rangle + b = 0\,.$$

$$\langle \boldsymbol{w}, \boldsymbol{x}_a \rangle + b - r\frac{\langle \boldsymbol{w}, \boldsymbol{w} \rangle}{\|\boldsymbol{w}\|} = 0\,.$$

$$r = \frac{1}{\|\boldsymbol{w}\|}\,.$$

$$\max_{\boldsymbol{w},b} \quad \frac{1}{\|\boldsymbol{w}\|}$$
$$\text{subject to } y_n(\langle \boldsymbol{w}, \boldsymbol{x}_n \rangle + b) \geqslant 1 \quad \text{for all} \quad n = 1, \ldots, N.$$

$$\min_{\boldsymbol{w},b} \quad \frac{1}{2}\|\boldsymbol{w}\|^2$$
$$\text{subject to } y_n(\langle \boldsymbol{w}, \boldsymbol{x}_n \rangle + b) \geqslant 1 \quad \text{for all} \quad n = 1, \ldots, N\,.$$

$$\max_{\boldsymbol{w},b,r} \quad \underbrace{r}_{\textit{margin}}$$
$$\text{subject to} \quad \underbrace{y_n(\langle \boldsymbol{w}, \boldsymbol{x}_n \rangle + b) \geqslant r}_{\textit{data fitting}}, \quad \underbrace{\|\boldsymbol{w}\| = 1}_{\textit{normalization}}, \quad r > 0\,, \tag{12.20}$$

is equivalent to scaling the data, such that the margin is unity:

$$\min_{\boldsymbol{w},b} \quad \underbrace{\frac{1}{2}\|\boldsymbol{w}\|^2}_{\textit{margin}}$$
$$\text{subject to} \quad \underbrace{y_n(\langle \boldsymbol{w}, \boldsymbol{x}_n \rangle + b) \geqslant 1}_{\textit{data fitting}}\,. \tag{12.21}$$

$$\max_{\boldsymbol{w}',b,r} \quad r^2$$

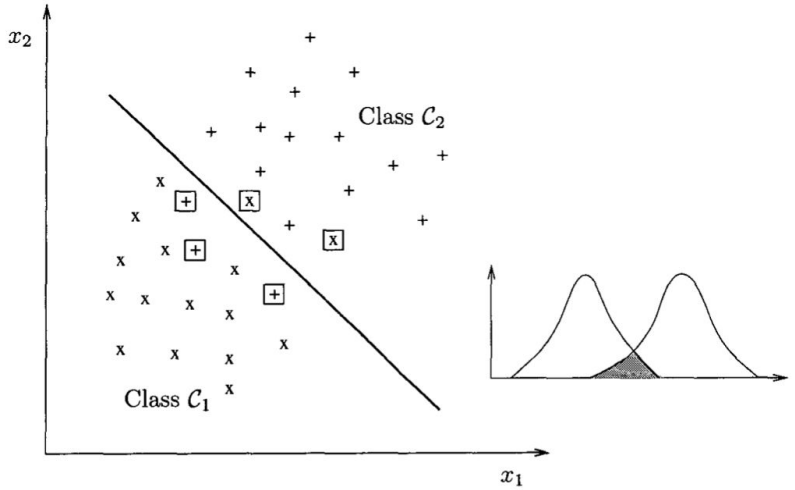
$$\text{subject to} \quad y_n \left(\left\langle \frac{\boldsymbol{w}'}{\|\boldsymbol{w}'\|}, \boldsymbol{x}_n \right\rangle + b \right) \geqslant r, \quad r > 0\,. \tag{12.22}$$

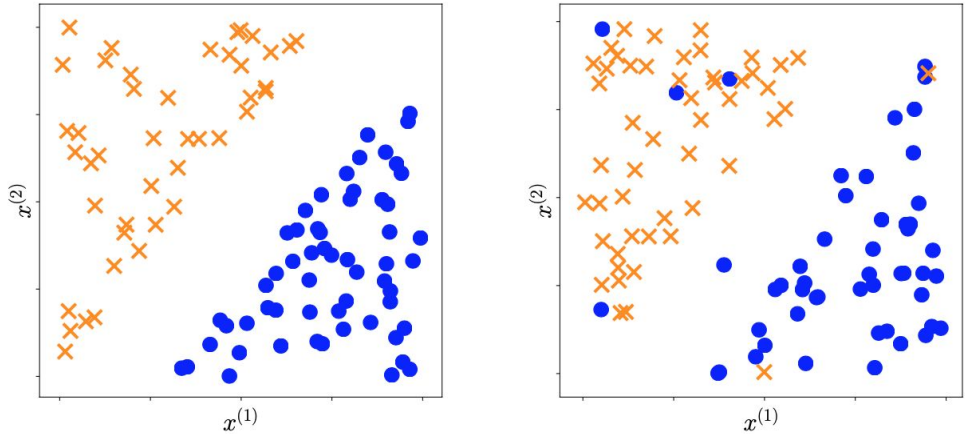
$$\max_{\boldsymbol{w}',b,r} \quad r^2$$

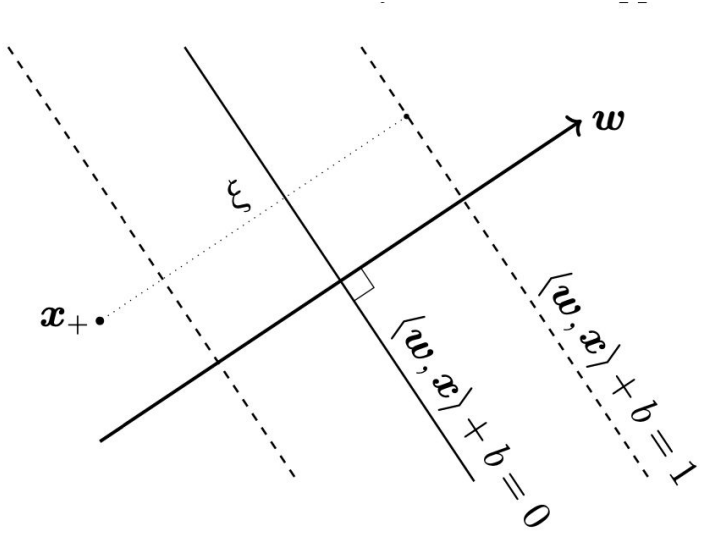
$$\text{subject to} \quad y_n \left(\left\langle \underbrace{\frac{\boldsymbol{w}'}{\|\boldsymbol{w}'\| \, r}}_{\boldsymbol{w}''}, \boldsymbol{x}_n \right\rangle + \underbrace{\frac{b}{r}}_{b''} \right) \geqslant 1, \quad r > 0$$

$$\|\boldsymbol{w}''\| = \left\| \frac{\boldsymbol{w}'}{\|\boldsymbol{w}'\| \, r} \right\| = \frac{1}{r} \cdot \left\| \frac{\boldsymbol{w}'}{\|\boldsymbol{w}'\|} \right\| = \frac{1}{r} \, .$$

$$\begin{aligned} \max_{\boldsymbol{w}'', b''} \quad & \frac{1}{\|\boldsymbol{w}''\|^2} \\ \text{subject to} \quad & y_n \left(\langle \boldsymbol{w}'', \boldsymbol{x}_n \rangle + b'' \right) \geqslant 1 \, . \end{aligned}$$


x_2
Class $\mathcal{C}_2$
Class $\mathcal{C}_1$
x_1


$x^{(2)}$
$x^{(1)}$
$x^{(2)}$
$x^{(1)}$


w
ξ
x_+
$\langle w, x \rangle + b = 1$
$\langle w, x \rangle + b = 0$

$$\begin{aligned} \min_{\boldsymbol{w},b,\boldsymbol{\xi}} \quad & \frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_{n=1}^{N}\xi_n \\ \text{subject to} \quad & y_n(\langle \boldsymbol{w}, \boldsymbol{x}_n \rangle + b) \geqslant 1 - \xi_n \\ & \xi_n \geqslant 0 \end{aligned}$$

$$\mathfrak{L}(\boldsymbol{w}, b, \xi, \alpha, \gamma) = \frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_{n=1}^{N}\xi_n \tag{12.34}$$

$$\underbrace{-\sum_{n=1}^{N}\alpha_n(y_n(\langle \boldsymbol{w}, \boldsymbol{x}_n\rangle + b) - 1 + \xi_n)}_{\text{constraint (12.26b)}} \underbrace{-\sum_{n=1}^{N}\gamma_n\xi_n}_{\text{constraint (12.26c)}} .$$

$$\frac{\partial \mathfrak{L}}{\partial \boldsymbol{w}} = \boldsymbol{w}^\top - \sum_{n=1}^{N} \alpha_n y_n \boldsymbol{x}_n{}^\top ,$$

$$\frac{\partial \mathfrak{L}}{\partial b} = \sum_{n=1}^{N} \alpha_n y_n ,$$

$$\frac{\partial \mathfrak{L}}{\partial \xi_n} = C - \alpha_n - \gamma_n .$$

$$\boldsymbol{w} = \sum_{n=1}^{N} \alpha_n y_n \boldsymbol{x}_n ,$$

$$\mathfrak{D}(\xi, \alpha, \gamma) = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} y_i y_j \alpha_i \alpha_j \left\langle \boldsymbol{x}_i, \boldsymbol{x}_j \right\rangle - \sum_{i=1}^{N} y_i \alpha_i \left\langle \sum_{j=1}^{N} y_j \alpha_j \boldsymbol{x}_j, \boldsymbol{x}_i \right\rangle$$
$$+ C \sum_{i=1}^{N} \xi_i - b \sum_{i=1}^{N} y_i \alpha_i + \sum_{i=1}^{N} \alpha_i - \sum_{i=1}^{N} \alpha_i \xi_i - \sum_{i=1}^{N} \gamma_i \xi_i \,.$$

$$\mathfrak{D}(\xi, \alpha, \gamma) = -\frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} y_i y_j \alpha_i \alpha_j \left\langle \boldsymbol{x}_i, \boldsymbol{x}_j \right\rangle + \sum_{i=1}^{N} \alpha_i + \sum_{i=1}^{N} (C - \alpha_i - \gamma_i) \xi_i \,.$$

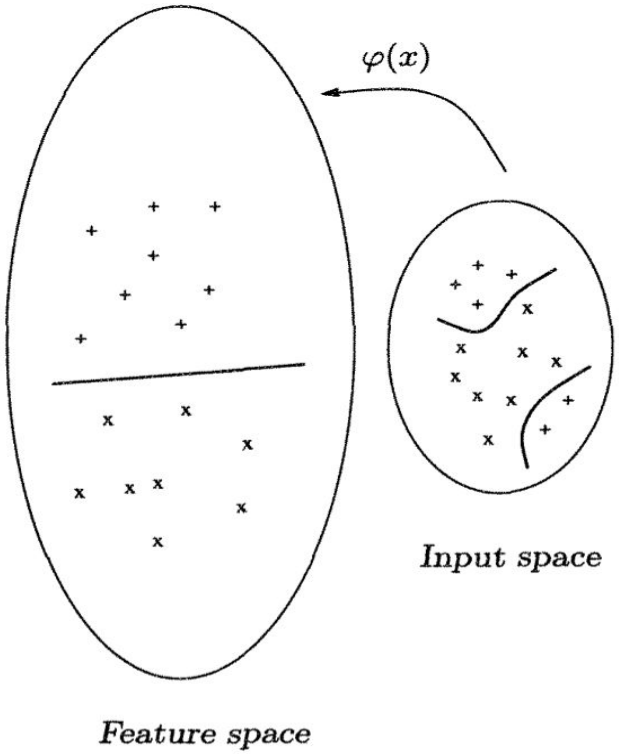
$$\begin{aligned}
\min_{\boldsymbol{\alpha}} \quad & \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} y_i y_j \alpha_i \alpha_j \left\langle \boldsymbol{x}_i, \boldsymbol{x}_j \right\rangle - \sum_{i=1}^{N} \alpha_i \\
\text{subject to} \quad & \sum_{i=1}^{N} y_i \alpha_i = 0 \\
& 0 \leqslant \alpha_i \leqslant C \quad \text{for all} \quad i = 1, \ldots, N \,.
\end{aligned} \tag{12.41}$$

$$K(x,z) = \sum_{i=1}^{n_{\mathcal{H}}} \lambda_i \phi_i(x) \phi_i(z),$$

Mercer's condition requires that

$$\int K(x,z) g(x) g(z) dx dz \geq 0$$

$$k(\boldsymbol{x}_i, \boldsymbol{x}_j) = \langle \boldsymbol{\phi}(\boldsymbol{x}_i), \boldsymbol{\phi}(\boldsymbol{x}_j) \rangle_{\mathcal{H}} \ .$$



$$y(x) = \text{sign}[w^T \varphi(x) + b]$$

$$\min_{w,b,\xi} J_{\mathrm{P}}(w,\xi) = \frac{1}{2}w^T w + c\sum_{k=1}^{N}\xi_k$$

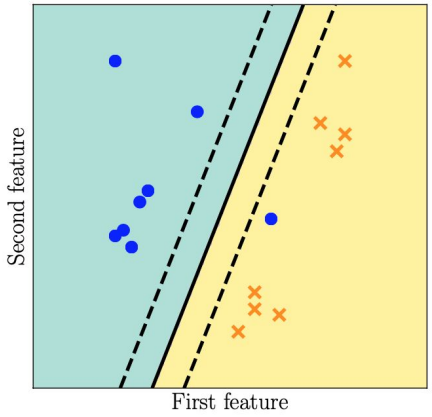
$$\text{such that} \quad y_k[w^T\varphi(x_k)+b] \geq 1-\xi_k, \qquad k=1,...,N$$

$$\xi_k \geq 0, \qquad k=1,...,N.$$

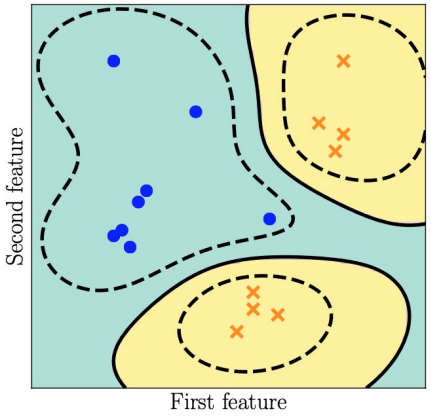
$$\max_{\alpha} J_{\mathrm{D}}(\alpha) = -\frac{1}{2}\sum_{k,l=1}^{N} y_k y_l\, K(x_k,x_l)\,\alpha_k\alpha_l + \sum_{k=1}^{N}\alpha_k$$

$$\text{such that} \quad \sum_{k=1}^{N}\alpha_k y_k = 0$$

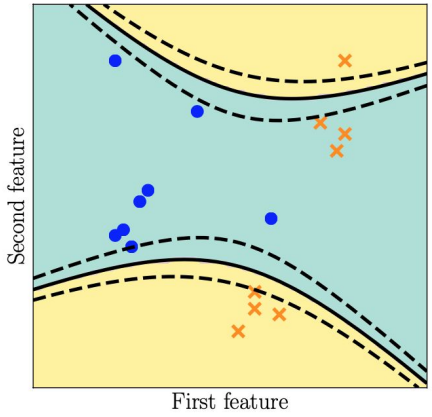
$$0 \leq \alpha_k \leq c, \; k=1,...,N.$$

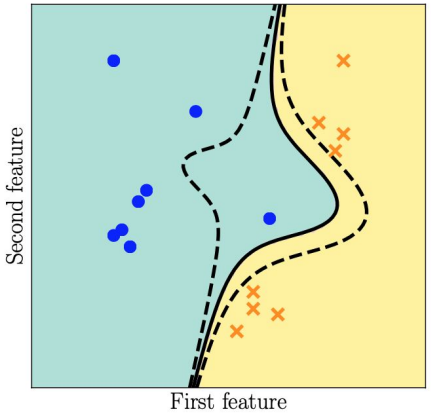


(a) SVM with linear kernel



(b) SVM with RBF kernel





Thank you for your attention!