Mini-course on Kernel Techniques

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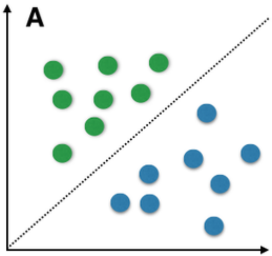
Idea of featurization: in classification



Decision surface:

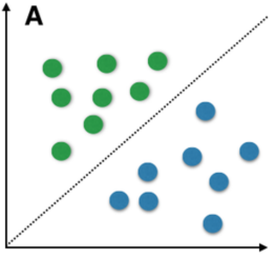
$$\{\mathbf{x} : \langle \boldsymbol{\beta}, \mathbf{x} \rangle = 0\} \Rightarrow$$

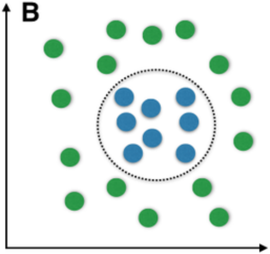
classes:

$$\{\mathbf{x} : \langle \boldsymbol{\beta}, \mathbf{x} \rangle \geq 0\} \qquad \{\mathbf{x} : \langle \boldsymbol{\beta}, \mathbf{x} \rangle < 0\} .$$

Idea of featurization: in classification

Idealized situation (Stylistic) real world





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Featurization – continued

On the ellipse

$$\left\{\mathbf{x} : \frac{(x_1 - c_1)^2}{a^2} + \frac{(x_2 - c_2)^2}{b^2} = 1\right\}$$

Featurization – continued

On the ellipse, outside

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Featurization – continued

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With polynomial feature: $\boxed{\varphi(\mathbf{x}) = (x_1^2, x_1, 1, x_2^2, x_2)}$:

- Decision surface: $\{\mathbf{x} : \langle \beta, \varphi(\mathbf{x}) \rangle = 0\}$.

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Quadratic & polynomial features

Still in $\mathbb{R}^2$:

$$\varphi(\mathbf{x}) = \left(x_1^2, \sqrt{2}x_1x_2, x_2^2\right),$$

$$\boxed{\langle \varphi(\mathbf{x}), \varphi(\mathbf{x}') \rangle} = ?$$

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$\langle\mathbf{x}, \mathbf{x}'\rangle^d = \langle\varphi(\mathbf{x}), \varphi(\mathbf{x}')\rangle$: $\varphi(\mathbf{x}) =$ d-order polynomial. $\Rightarrow$ Explicit computation would be computationally intense! $\boxed{\varphi = ?}$

Why kernels/RKHSs?

Key idea

$k(x, x') = \langle \varphi(x), \varphi(x') \rangle_{\mathcal{H}}.$

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   - $\mathcal{H}_k \subset \mathbb{R}^{\mathcal{X}}$: extension to vector-valued setting $\exists$ ($\mathcal{H}_k \subset \mathcal{H}^{\mathcal{X}}$, $k(x, x') \in \mathcal{L}(\mathcal{H})$; dependency of output coordinates).

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5. goes far beyond supervised learning (dimensionality reduction: KPCA, KCCA; information theoretical estimators: MMD, HSIC, KSD, ...) $\Rightarrow$ latter (KSD): Wednesday.

Content: supervised learning

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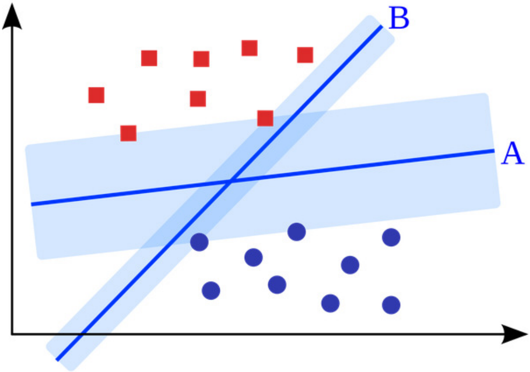
  3. non-linear close-to separability:
     - linearity after featurization $\Rightarrow$ kernel, RKHS, representer theorem.
- Regression (SVMR $\xrightarrow{\text{spec.}}$ kernel ridge regression):
  - quadratic cost + quadratic regularization,
  - an other application of the representer theorem.

(Towards) linear SVMC

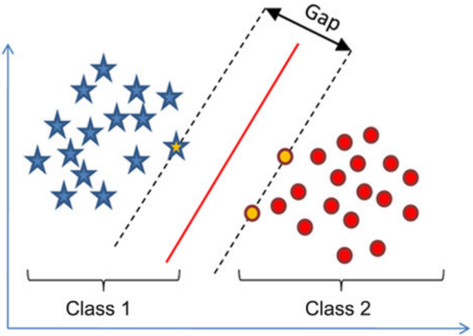
Idea of SVMC

- Task: binary classification.
- Given: training set $\{(\mathbf{x}_i, y_i)\}_{i=1}^n \in \mathbb{R}^p \times \{-1, 1\}$, linearly separable.
- Question: Which separating line is the 'best'?



SVMC

Answer/intuition: the one with the largest margin.



Needed

hyperplane, margin

Hyperplanes

- Hyperplane going through the origin: with normal vector $\beta \in \mathbb{R}^p$

$$H_{\beta} := \{\mathbf{x} \in \mathbb{R}^p \ : \ \langle \beta, \mathbf{x} \rangle = 0\}.$$

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- Hyperplane: with normal vector $\boldsymbol{\beta} \in \mathbb{R}^p$ and offset $\beta_0 \in \mathbb{R}$

$$H_{\boldsymbol{\beta},\beta_0} := \{\mathbf{x} \in \mathbb{R}^p \; : \; \langle \boldsymbol{\beta}, \mathbf{x} \rangle + \beta_0 = 0\}.$$

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- The 2 sides of the hyperplane:

$$H^{+}_{\beta,\beta_0} := \{\mathbf{x} \in \mathbb{R}^p \ : \ \langle \beta, \mathbf{x} \rangle + \beta_0 > 0\},$$
$$H^{-}_{\beta,\beta_0} := \{\mathbf{x} \in \mathbb{R}^p \ : \ \langle \beta, \mathbf{x} \rangle + \beta_0 < 0\}.$$

We will use H_{β,β_0}

Hyperplane: properties

Recall:

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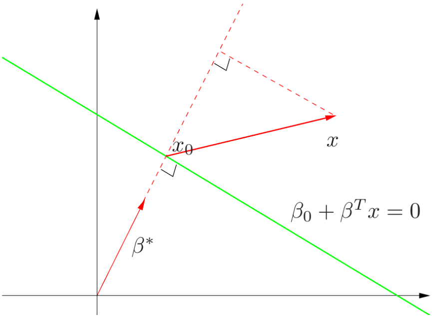

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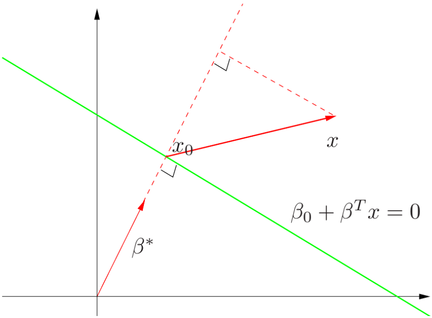
$$\langle \beta^*, \mathbf{x} - \mathbf{x}_0 \rangle = \left\langle \frac{\beta}{\|\beta\|_2}, \mathbf{x} \right\rangle - \left\langle \frac{\beta}{\|\beta\|_2}, \mathbf{x}_0 \right\rangle$$



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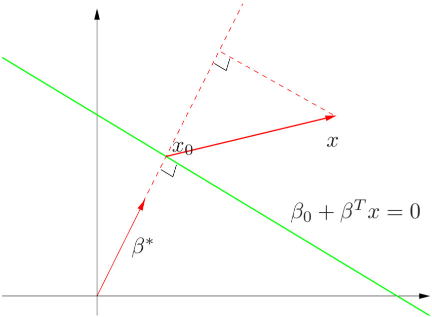

Optimization problem for max-margin hyperplane

Wanted

$y_i = +1 \Rightarrow \langle \boldsymbol{\beta}, \mathbf{x}_i \rangle + \beta_0 > 0$; $y_i = -1 \Rightarrow \langle \boldsymbol{\beta}, \mathbf{x}_i \rangle + \beta_0 < 0$.

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SVMC: hard vs soft

- Hard classification :
  - decision: $\hat{y}(\mathbf{x}) = \text{sign}(\langle \boldsymbol{\beta}, \mathbf{x} \rangle + \beta_0)$.
  - objective:

$$\min_{\boldsymbol{\beta}, \beta_0} \frac{1}{2} \|\boldsymbol{\beta}\|_2^2 \ \text{ s.t. } \ y_i \left(\langle \boldsymbol{\beta}, \mathbf{x}_i \rangle + \beta_0 \right) \geq 1, \forall i \in [n].$$

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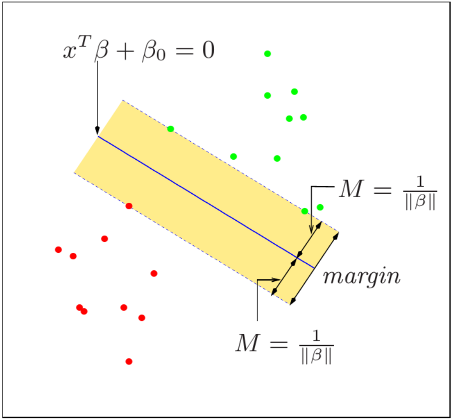
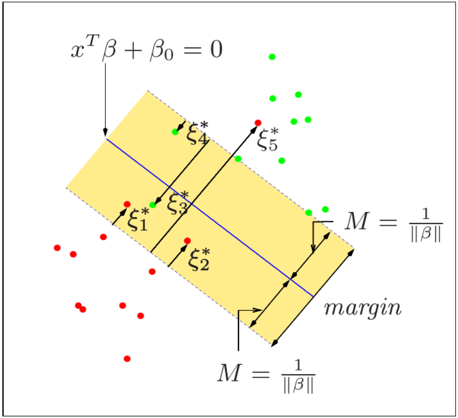
- Soft classification objective ($C > 0$):

$$\min_{\boldsymbol{\beta}, \beta_0, \boldsymbol{\xi}} \frac{1}{2} \|\boldsymbol{\beta}\|_2^2 + C \sum_{i=1}^{n} \xi_i \;\text{ s.t. }\; y_i \left(\langle \boldsymbol{\beta}, \mathbf{x}_i \rangle + \beta_0 \right) \geq 1 - \overbrace{\xi_i ,}^{\text{slack variables}} \xi_i \geq 0, \; \forall i \in [n].$$

  Linear penalty on misclassification.

Hard vs soft SVMC: visual illustration ($\|\cdot\| := \|\cdot\|_2$)





Note on the objective of soft SVMC

$$\min_{\boldsymbol{\beta},\beta_0,\boldsymbol{\xi}} \frac{1}{2}\|\boldsymbol{\beta}\|_2^2 + C\sum_{i=1}^{n}\xi_i \ \text{ s.t. } \ y_i\left(\langle\boldsymbol{\beta},\mathbf{x}_i\rangle + \beta_0\right) \geq 1 - \xi_i,\ \xi_i \geq 0,\ \forall i \in [n]$$

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where $h(u) = \max(1-u, 0)$ is the hinge loss.

Note on the objective of soft SVMC – continued

The hinge loss is the convex envelope of the zero-one loss:

$$z(u) = I_{\mathbb{R}_{<0}}(u), \qquad u = y_i f(x_i),$$
$$h(u) = \max(1 - u, 0).$$

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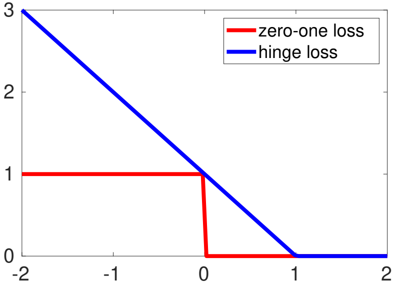


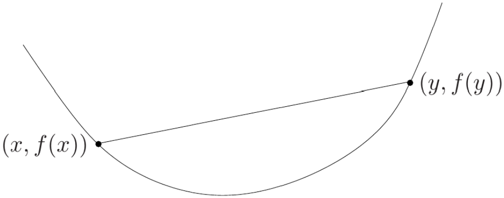
Computation

Convex optimization, duality.

Convex function

- A function $f : \mathbb{R}^d \to \mathbb{R}$ is called convex if
  1. $\mathrm{dom}(f) \coloneqq \{\mathbf{x} \in \mathbb{R}^d : f(\mathbf{x}) \text{ is defined}\}$ is convex, and
  2. for all $\mathbf{x}, \mathbf{y} \in \mathrm{dom}(f)$ and $\alpha \in [0, 1]$

$$f(\alpha\mathbf{x} + (1-\alpha)\mathbf{y}) \leq \alpha f(\mathbf{x}) + (1-\alpha) f(\mathbf{y}).$$



Convex and concave functions

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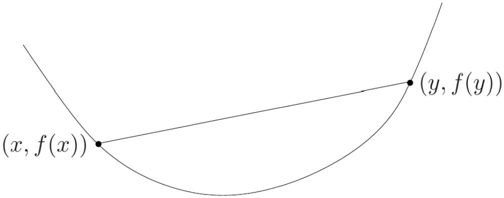

- f is called concave if $-f$ is convex.

Convex and concave functions, affine ones

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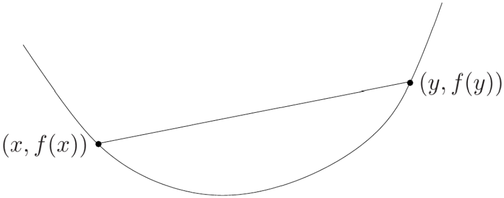

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- Affine functions ($\mathbf{x} \mapsto \langle \mathbf{w}, \mathbf{x} \rangle + b$) are both convex and concave.

Optimization

- Task:

$$\begin{aligned} \min_{\mathbf{x} \in \mathbb{R}^d} \quad & f_0(\mathbf{x}) \\ \text{s.t.} \quad & f_i(\mathbf{x}) \leq 0, \; i \in [m], \\ & h_j(\mathbf{x}) = 0, \; j \in [p]. \end{aligned}$$

$p^* :=$ optimal value of this problem. Assume: $\mathcal{D} := \left(\cap_{i=0}^m \operatorname{dom}(f_i)\right) \cap \left(\cap_{j \in [p]} \operatorname{dom}(h_j)\right) \neq \emptyset$.

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- Lagrangian function: $\operatorname{dom}(L) = \mathcal{D} \times \mathbb{R}^m \times \mathbb{R}^p$

$$L(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\nu}) = f_0(\mathbf{x}) + \sum_{i\in[m]} \lambda_i f_i(\mathbf{x}) + \sum_{j\in[p]} \nu_j h_j(\mathbf{x}).$$

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  dual variables: $\boldsymbol{\lambda} = (\lambda_i)_{i=1}^m \in \mathbb{R}^m$, $\boldsymbol{\nu} = (\nu_j)_{j=1}^p \in \mathbb{R}^p$.

Lagrange dual function

Consider for all $\boldsymbol{\lambda} \in \mathbb{R}^m$ and $\boldsymbol{\nu} \in \mathbb{R}^p$, the 'minimum' of the Lagrangian:

$$g(\boldsymbol{\lambda}, \boldsymbol{\nu}) := \inf_{\mathbf{x} \in \mathcal{D}} L(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\nu}) = \inf_{\mathbf{x} \in \mathcal{D}} \left(f_0(\mathbf{x}) + \sum_{i \in [m]} \lambda_i f_i(\mathbf{x}) + \sum_{j \in [p]} \nu_j h_j(\mathbf{x}) \right).$$

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Lagrange dual function, Lagrange dual problem

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- Lagrange dual problem: best lower bound with the Lagrange function

$$\begin{aligned} \max_{\substack{\boldsymbol{\lambda} \in \mathbb{R}^m, \\ \boldsymbol{\nu} \in \mathbb{R}^p}} \quad & g(\boldsymbol{\lambda}, \boldsymbol{\nu}) \\ \text{s.t.} \quad & \boldsymbol{\lambda} \geq \mathbf{0}_m. \end{aligned}$$

Dual optimal: $(\boldsymbol{\lambda}^*, \boldsymbol{\nu}^*)$; optimal value d^*. Above $\Rightarrow$ $d^* \leq p^*$.

KKT conditions for convex problems: optimality

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i.e., (1)-(2): $\tilde{\mathbf{x}}$ is primal feasible; (3): dual feasibility; (4): complementary slackness; (5): $\tilde{\mathbf{x}}$ minimizes $L(\cdot, \tilde{\boldsymbol{\lambda}}, \tilde{\boldsymbol{\nu}})$.

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Let us deploy this statement to our soft SVMC!

Soft SVMC: back to optimization

Objective:

$$\min_{\boldsymbol{\beta},\beta_0,\boldsymbol{\xi}} \frac{1}{2}\|\boldsymbol{\beta}\|_2^2 + C\sum_{i=1}^{n}\xi_i, \text{ s.t. } y_i\left(\langle\boldsymbol{\beta},\mathbf{x}_i\rangle + \beta_0\right) \geq 1-\xi_i,\ \xi_i \geq 0 \quad (\forall i) \Leftrightarrow$$

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Standard convex optimization form:

$$\begin{aligned}
\min_{(\boldsymbol{\beta},\beta_0,\boldsymbol{\xi})\in\mathbb{R}^{p+1+n}} \quad & f_0(\boldsymbol{\beta},\beta_0,\boldsymbol{\xi}) := \frac{1}{2}\|\boldsymbol{\beta}\|_2^2 + C\sum_{i=1}^{n}\xi_i \\
\text{s.t.} \quad & f_i(\boldsymbol{\beta},\beta_0,\boldsymbol{\xi}) := 1-\xi_i-y_i\left(\langle\boldsymbol{\beta},\mathbf{x}_i\rangle+\beta_0\right)\leq 0,\ i\in[n], \\
& f_i(\boldsymbol{\beta},\beta_0,\boldsymbol{\xi}) := -\xi_i \leq 0,\ i\in\{n+1,\ldots,n+n\}.
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\end{aligned}$$

KKT conditions kick in

$\Leftarrow$ f_i-s are convex and differentiable, no equality constraints.

Soft SVMC: continued

Lagrangian function: with $\alpha_i \geq 0, \mu_i \geq 0$ $(\forall i)$

$$L(\boldsymbol{\beta}, \beta_0, \boldsymbol{\xi}; \boldsymbol{\alpha}, \boldsymbol{\mu}) = \text{objective} + \text{Lagrangian multipliers} \times \text{conditions}$$
$$= \frac{1}{2} \|\boldsymbol{\beta}\|_2^2 + C \sum_{i=1}^{n} \xi_i - \sum_{i=1}^{n} \alpha_i \left[y_i \left(\langle \boldsymbol{\beta}, \mathbf{x}_i \rangle + \beta_0 \right) - 1 + \xi_i \right] - \sum_{i=1}^{n} \mu_i \xi_i .$$

Solving for $\frac{\partial L}{\partial \text{primal}} = 0$, we get ...

Soft SVMC: continued

$$L(\boldsymbol{\beta}, \beta_0, \boldsymbol{\xi}; \boldsymbol{\alpha}, \boldsymbol{\mu}) =$$
$$= \frac{1}{2}\|\boldsymbol{\beta}\|_2^2 + C\sum_{i=1}^n \xi_i - \sum_{i=1}^n \alpha_i \left[y_i\left(\langle \boldsymbol{\beta}, \mathbf{x}_i\rangle + \beta_0\right) - 1 + \xi_i\right] - \sum_{i=1}^n \mu_i \xi_i.$$

Optimality equations:

$$\mathbf{0} = \frac{\partial L}{\partial \boldsymbol{\beta}} = \boldsymbol{\beta} - \sum_{i=1}^n \alpha_i y_i \mathbf{x}_i \quad (\boldsymbol{\beta} \leftrightarrow \boldsymbol{\alpha}),$$
$$0 = \frac{\partial L}{\partial \beta_0} = \sum_{i=1}^n \alpha_i y_i,$$
$$0 = \frac{\partial L}{\partial \xi_i} = C - \alpha_i - \mu_i, \ \forall i \in [n].$$

Plugging these equations back to L, we have ...

Soft SVMC: after a bit of calculation

- Lagrange dual problem (QP):

$$\max_{\boldsymbol{\alpha}\in\mathbb{R}^n} \underbrace{\sum_{i=1}^{n}\alpha_i - \frac{1}{2}\sum_{i,j=1}^{n}\alpha_i\alpha_j y_i y_j \boxed{\langle \mathbf{x}_i, \mathbf{x}_j\rangle}}_{\text{quadratic in } \boldsymbol{\alpha}}, \text{ s.t. } \underbrace{0 \le \alpha_i \le C\ (\forall i), \sum_{i=1}^{n}\alpha_i y_i = 0}_{\text{linear in } \boldsymbol{\alpha}}.$$

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- β_0 recovery: from complementary slackness, i.e. when $\alpha_i \neq 0$ (support vectors), $y_i\left(\langle \boldsymbol{\beta}, \mathbf{x}_i\rangle + \beta_0\right) - 1 = 0$ needs to hold.

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- Decision:

$$\hat{y}(\mathbf{x}) = \operatorname{sign}(\langle \boldsymbol{\beta}, \mathbf{x}\rangle + \beta_0) = \operatorname{sign}\left(\left\langle \sum_{i\in[n]}\alpha_i y_i \mathbf{x}_i, \mathbf{x}\right\rangle + \beta_0\right)$$

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(Towards) nonlinear SVMC

If linear separability does not hold

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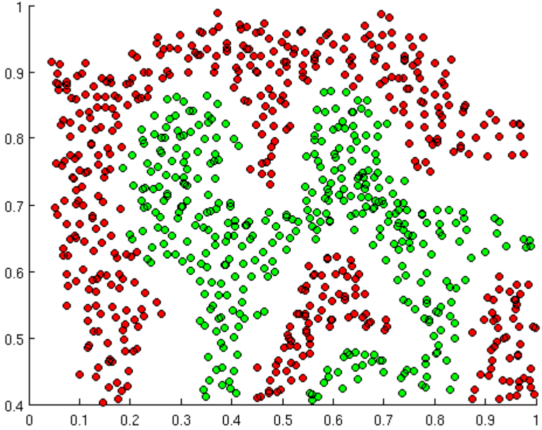
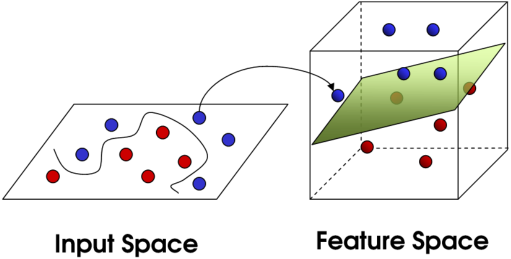


If linear separability does not hold: kernel trick



Nonlinear SVMC

- Linear SVMC (dual):

$$\max_{\boldsymbol{\alpha}} \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle, \text{ s.t. } \sum_{i=1}^{n} \alpha_i y_i = 0,\ 0 \le \alpha_i \le C\ (\forall i).$$

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- Nonlinear SVMC (primal):

$$\min_{f\in\mathcal{H}_k, \boldsymbol{\xi}} \frac{1}{2}\|f\|_{\mathcal{H}_k}^2 + C\sum_{i=1}^{n} \xi_i, \text{ s.t. } y_i f(x_i) \ge 1 - \xi_i,\ \xi_i \ge 0,\ \forall i.$$

What is $\mathcal{H}_k$? Note: '$+\beta_0$' also works.

Kernel examples on $\mathbb{R}^d$ ($c \geq 0$, $p \in \mathbb{Z}^+$)

$$k_p(\mathbf{x}, \mathbf{y}) = (\langle \mathbf{x}, \mathbf{y} \rangle + c)^p$$

Kernel examples on $\mathbb{R}^d$ ($\gamma > 0$, $c \geq 0$, $p \in \mathbb{Z}^+$)

$$k_p(\mathbf{x},\mathbf{y}) = (\langle \mathbf{x},\mathbf{y}\rangle + c)^p, \qquad k_G(\mathbf{x},\mathbf{y}) = e^{-\gamma\|\mathbf{x}-\mathbf{y}\|_2^2},$$

$$k_e(\mathbf{x},\mathbf{y}) = e^{-\gamma\|\mathbf{x}-\mathbf{y}\|_2}, \qquad k_L(\mathbf{x},\mathbf{y}) = e^{-\gamma\|\mathbf{x}-\mathbf{y}\|_1},$$

$$k_C(\mathbf{x},\mathbf{y}) = \frac{1}{1+\gamma\left\|\mathbf{x}-\mathbf{y}\right\|_2^2}, \qquad k_{\tilde{e}}(\mathbf{x},\mathbf{y}) = e^{\gamma\langle \mathbf{x},\mathbf{y}\rangle}.$$

Kernel examples on $\mathbb{R}^d$ ($\gamma, \sigma, v > 0$, $c \geq 0$, $p \in \mathbb{Z}^+$)

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Or the flexible Matérn family:

$$k_M(\mathbf{x},\mathbf{y}) = \frac{2^{1-v}}{\Gamma(v)}\left(\frac{\sqrt{2v}\,\|\mathbf{x}-\mathbf{y}\|_2}{\sigma}\right)^{v} K_v\left(\frac{\sqrt{2v}\,\|\mathbf{x}-\mathbf{y}\|_2}{\sigma}\right),$$

where

- K_v: modified Bessel function of the second kind of order v,
- Specific cases: For $v=\frac{1}{2}$ one gets $k(\mathbf{x},\mathbf{y}) = e^{-\frac{\|\mathbf{x}-\mathbf{y}\|_2}{\sigma}}$. Gaussian kernel: $v \to \infty$.

Some kernel-enriched domains: $(\mathcal{X}, k)$

- Strings [Watkins, 1999, Lodhi et al., 2002, Leslie et al., 2002, Kuang et al., 2004, Leslie and Kuang, 2004, Saigo et al., 2004, Cuturi and Vert, 2005],
- time series [Rüping, 2001, Cuturi et al., 2007, Cuturi, 2011, Király and Oberhauser, 2019],
- trees [Collins and Duffy, 2001, Kashima and Koyanagi, 2002],
- groups and specifically rankings [Cuturi et al., 2005, Jiao and Vert, 2016],
- sets [Haussler, 1999, Gärtner et al., 2002, Balanca and Herbin, 2012, Fellmann et al., 2024], probability distributions [Berlinet and Thomas-Agnan, 2004, Hein and Bousquet, 2005, Smola et al., 2007, Sriperumbudur et al., 2010],
- various generative models [Jaakkola and Haussler, 1999, Tsuda et al., 2002, Seeger, 2002, Jebara et al., 2004],
- fuzzy domains [Guevara et al., 2017], or
- graphs [Kondor and Lafferty, 2002, Gärtner et al., 2003, Kashima et al., 2003, Borgwardt and Kriegel, 2005, Shervashidze et al., 2009, Vishwanathan et al., 2010, Kondor and Pan, 2016, Bai et al., 2020, Borgwardt et al., 2020, Schulz et al., 2022, Nikolentzos and Vazirgiannis, 2023].

Kernel (generalization of $\mathbf{a}^\top \mathbf{b}$), RKHS

Our assumption

input space: $\mathcal{X}$ is a set.

Def-1 (feature): $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is called **kernel** if $\exists$ feature map $\varphi : \mathcal{X} \to \mathcal{H}$(ilbert) s.t.

$$k(x, x') = \langle \varphi(x), \varphi(x') \rangle_{\mathcal{H}}, \quad x, x' \in \mathcal{X}.$$

Def-2 (reproducing kernel):

- $\mathcal{H} \subset \mathbb{R}^{\mathcal{X}}$: Hilbert space.
- $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a r.k. of $\mathcal{H}$ if for $\forall x \in \mathcal{X}, f \in \mathcal{H}$:
  1. $k(\cdot, x) \in \mathcal{H}$: 'generators',
  2. $f(x) = \langle f, k(\cdot, x)\rangle_{\mathcal{H}}$: reproducing property.

Kernel, RKHS – continued

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Remarks

1. Specifically, $k(x, y) = \langle k(\cdot, x), k(\cdot, y) \rangle_{\mathcal{H}}$;
   note: $k(\cdot, x) =:$ canonical feature map.
2. Reproducing property $\Rightarrow$ computational tractability.

Kernel, RKHS – continued

- Def-3 (Gram matrix):
  - $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ symmetric function.
  - k is called positive definite if for $\forall n \in \mathbb{Z}^+, (x_i)_{i=1}^n \in \mathcal{X}^n$

$$\mathbb{R}^{n\times n} \ni \mathbf{G} = [k(x_i, x_j)]_{i,j=1}^n \succeq \mathbf{0}_{n\times n}.$$

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Benefits

1. Optimization advantage: $\exists(\mathbf{G} + \lambda\mathbf{I})^{-1}$.
2. Computation: reduces to linear algebra.

Kernel, RKHS – continued

Def-4 (evaluation):

- $\mathcal{H} \subset \mathbb{R}^{\mathcal{X}}$: Hilbert space.
- Let $\delta_x : f \in \mathcal{H} \mapsto f(x) \in \mathbb{R}$, with $x \in \mathcal{X}$.
- $\mathcal{H}$ is called RKHS if for $\forall x \in \mathcal{X}$, δ_x is continuous.

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Strong notion of convergence: $f_n \to f \Rightarrow$ for $\forall x \in \mathcal{X}$, $f_n(x) \to f(x)$.

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How do we construct kernels?

Kernel factory

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  2. Cone. If $k_m : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ kernel, $\alpha_m \geq 0$ ($m = 1, \ldots, M$), then

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\end{aligned}$$

Example: $\oplus_{m=1}^{M} \mathbb{R} = \mathbb{R}^M$.

Kernel factory – continued

4. **Product.** If $(k_m)_{m=1}^M$ are kernels on $(\mathcal{X}_m)_{m=1}^M$, then

$$\left(\otimes_{m=1}^M k_m\right)\left(\left(x_1, \ldots, x_M\right), \left(x_1', \ldots, x_M'\right)\right) = \prod_{m=1}^M k_m\left(x_m, x_m'\right).$$

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- Thus, $(k_m)_{m=1}^M:\mathcal{X}\times\mathcal{X}\to\mathbb{R}$ kernels $\Rightarrow\prod_{m=1}^M k_m(x,x')$: kernel on $\mathcal{X}$.
- Consequence ($\gamma\geq 0$, $p\in\mathbb{Z}^+$):

$$k(\mathbf{x},\mathbf{y})=\left(\langle\mathbf{x},\mathbf{y}\rangle_2+\gamma\right)^p$$

is a kernel.

Kernel factory

6. Limit. If $(k_n)_{n\in\mathbb{N}}$ are kernels on $\mathcal{X}$, then

$$k(x,x') := \lim_{n\to\infty} k_n(x,x')$$

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$$k(\mathbf{x},\mathbf{y}) = e^{\gamma\langle\mathbf{x},\mathbf{y}\rangle_2} = \sum_{n\in\mathbb{N}} \frac{\left(\gamma\langle\mathbf{x},\mathbf{y}\rangle_2\right)^n}{n!}$$

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Reason: polynomial kernel & limit rule.

Kernel factory – continued

7. Pre-post multiplication. k kernel on $\mathcal{X}$, $f : \mathcal{X} \to \mathbb{R}$, then

$$\tilde{k}(x, y) = f(x)k(x, y)f(y)$$

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Example (Gaussian kernel, $\gamma > 0$): previous example & new rule

$$k(\mathbf{x}, \mathbf{y}) = e^{-\gamma\|\mathbf{x}-\mathbf{y}\|_2^2}$$

by using $\|\mathbf{x} - \mathbf{y}\|_2^2 = \|\mathbf{x}\|_2^2 + \|\mathbf{y}\|_2^2 - 2\langle\mathbf{x}, \mathbf{y}\rangle$.

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Properties of k control that of $\mathcal{H}_k$

- k: bounded $[\sup_{x,y\in\mathcal{X}} k(x,y) \le C] \Rightarrow \forall f \in \mathcal{H}_k$ is bounded

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- k: analytic $\Rightarrow \forall f \in \mathcal{H}_k$ is analytic.

Representer theorem ⇒ finiteD parameterization!

- Given: $\{(x_i, y_i)\}_{i=1}^n$, say classification/regression.
- Goal:

$$J(f) = V(x_1, y_1, f(x_1), \ldots, x_n, y_n, f(x_n)) + r\left(\|f\|^2_{\mathcal{H}_k}\right) \to \min_{f \in \mathcal{H}_k},$$

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- Example:

$$V(\ldots) = \frac{1}{n}\sum_{i\in[n]} \max(1 - y_i f(x_i), 0) \quad \text{(soft classification)},$$

$$V(\ldots) = \frac{1}{n}\sum_{i\in[n]} [f(x_i) - y_i]^2 \quad \text{(regression-1)},$$

$$V(\ldots) = \frac{1}{n}\sum_{i\in[n]} |f(x_i) - y_i|_\epsilon \quad \text{(regression-2)},$$

with $|z|_\epsilon := \max(0, |z| - \epsilon)$, where $z \in \mathbb{R}$.

Representer theorem – continued

...then

- $\exists$ solution in the form:

$$\boxed{f^* = \sum_{i=1}^{n} \alpha_i k(\cdot, x_i)}, \quad \alpha_i \in \mathbb{R}.$$

- r: strictly increasing $\Rightarrow$ $\forall$ solution is of this form.
- Example: $r(z) = \lambda z$, $\lambda > 0$.

Representer theorem – proof

Objective

$$J(f) = V(x_1, y_1, f(x_1), \ldots, x_n, y_n, f(x_n)) + r\left(\|f\|^2_{\mathcal{H}_k}\right) \to \min_{f \in \mathcal{H}_k}.$$

Decompose & Pythagorean theorem:

$$\begin{aligned} S &= \operatorname{Span}\left(k(\cdot, x_i) \,:\, i \in [n]\right), \\ f &= f_S + f_\perp, \\ \|f\|^2_{\mathcal{H}_k} &= \|f_S\|^2_{\mathcal{H}_k} + \underbrace{\|f_\perp\|^2_{\mathcal{H}_k}}_{\geq 0} \geq \|f_S\|^2_{\mathcal{H}_k}. \end{aligned}$$

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- 1st term: depends on f_S only,
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  $f(x_i) = \langle f, k(\cdot, x_i)\rangle_{\mathcal{H}_k} = \langle f_S + f_\perp, k(\cdot, x_i)\rangle_{\mathcal{H}_k} = \langle f_S, k(\cdot, x_i)\rangle_{\mathcal{H}_k}$.
- 2nd term: can only decrease by neglecting $f_\perp$ ($r \nearrow$).

Regression: kernel ridge regression

Kernel ridge regression

- Given: $\{(x_i, y_i)\}_{i=1}^n$, $\mathcal{H} := \mathcal{H}_k$, $y_i \in \mathbb{R}$.
- Task ($\lambda > 0$):

$$J(f) = \frac{1}{n}\sum_{i=1}^{n}[y_i - f(x_i)]^2 + \lambda \|f\|_{\mathcal{H}}^2 \to \min_{f \in \mathcal{H}}.$$

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- Analytical solution:

$$f(x) = [k(x_1, x), \ldots, k(x_n, x)]\,(\mathbf{G} + \lambda n \mathbf{I}_n)^{-1}[y_1; \ldots; y_n],$$
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Question

How do we get this solution?

Kernel ridge regression

By the representer theorem

$$f = \sum_{i=1}^{n} a_i k(\cdot, x_i), \quad (a_i \in \mathbb{R}).$$

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Multiplying the objective by n, using the reproducing property:

$$\begin{aligned}
\tilde{J}(f) &= \sum_{j=1}^{n} \left[y_j - \langle f, k(\cdot, x_j) \rangle_{\mathcal{H}} \right]^2 + \lambda n \|f\|_{\mathcal{H}}^2 \\
&= \|\mathbf{y} - \mathbf{G}\mathbf{a}\|_2^2 + (\lambda n)\mathbf{a}^\top \mathbf{G}\mathbf{a} \\
&= \mathbf{y}^\top \mathbf{y} - 2\mathbf{y}^\top \mathbf{G}\mathbf{a} + \mathbf{a}^\top \left[\mathbf{G}^2 + (\lambda n)\mathbf{G} \right] \mathbf{a}.
\end{aligned}$$

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Solving $\mathbf{0} = \frac{\partial \tilde{J}}{\partial \mathbf{a}}$, one gets $\mathbf{a}^* = (\mathbf{G} + \lambda n \mathbf{I}_n)^{-1}\mathbf{y}$

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$$\frac{\partial \mathbf{a}^\top \mathbf{B}\mathbf{a}}{\partial \mathbf{a}} = \left(\mathbf{B} + \mathbf{B}^\top\right)\mathbf{a}, \quad \frac{\partial \mathbf{c}^\top \mathbf{a}}{\partial \mathbf{a}} = \mathbf{c}.$$

Summary

1. featurization idea.
2. SVMC:
    - max-margin principle,
    - optimization: duality, KKT conditions,
    - linear (hard/soft), non-linear,
    - kernels, RKHS ('any' data type).
3. representer theorem: finiteD parameterization.
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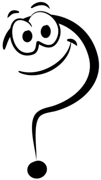

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