

Statistical Learning on Reproducing Kernel Hilbert Spaces

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Kernel-based learning algorithms

- Information technology related statistics— currently active, cross discipline research area.
- Kernel-based learning algorithms: SVM, kernel PCA, kernel ICA, kernel Fisher discriminant analysis, kernel SIR, etc.

convenient algorithm ^{kernelization} — — — → same type algorithm on an RKHS.

- Reproducing kernels (RKs) provide a convenient framework for efficient computation.
- RKHS lays a theoretical foundation for statistical inference: sparse approximation, regularization, Gauss-Markov prediction, Bayesics, likelihood criterion, etc.

Basic properties of RKHS

RKHS: Basics -1

- Consider a linear class \mathcal{H} of (real) functions $f(x)$ defined in a set E , forming a Hilbert space.
- **Definition** (Aronszajn, 1950, Trans. AMS). A real symmetric function $K(x, y)$ in $E \times E$ is called an **RK** of \mathcal{H} if
 - For every $x \in E$, $K(x, \cdot) \in \mathcal{H}$.
 - For every $x \in E$ and $f \in \mathcal{H}$, we have the reproducing property

$$\langle f(\cdot), K(x, \cdot) \rangle_{\mathcal{H}} = f(x).$$

- All kernels considered in this talk are real symmetric.
- The space \mathcal{H} is called an **RKHS**.

RKHS: Basics -2

RKHS \rightarrow RK

- For the **existence** of an RK, it is necessary and sufficient that for every $y \in E$, the evaluation functional, $\ell_y : f \rightarrow f(y)$, $f \in \mathcal{H}$, is a continuous functional.
- If an RK exists, it is **unique**.
- Riesz representation theory: $\ell_y(f) = \langle f, g_y \rangle_{\mathcal{H}}$. The **RK** is given by $K(x, y) = g_y(x)$.

RKHS: Basics -3

Positive definite kernel \rightarrow RKHS

- $K(x, y)$ is **positive definite** on $E \times E$ if, for all $x_1, \dots, x_n \in E$, the quadratic form in ξ_1, \dots, ξ_n : $\sum_{i,j=1}^n K(x_i, x_j) \xi_i \xi_j \geq 0$.
- To every positive definite kernel $K(x, y)$, there corresponds one and only one class of functions forming a Hilbert space and admitting K as an RK. (**existence and uniqueness**)
- Such a Hilbert space consists of functions of the form $\sum \alpha_i K(x, x_i)$ with norm

$$\left\| \sum \alpha_i K(x, x_i) \right\|_{\mathcal{H}}^2 = \sum_{i,j=1}^n K(x_i, x_j) \alpha_i \alpha_j.$$

RKHS: $\mathcal{H} = \text{closure}\{\sum \alpha_i K(x, x_i)\}$

RKHS: Basics -4

- **Restriction** of an RK to $E_1 \subset E$.

- ◊ $K_1(\cdot, \cdot) = K(\cdot, \cdot)|_{E_1 \times E_1}$: \mathcal{H}_1 with norm $\|f_1\|_{\mathcal{H}_1} = \inf_{\mathcal{F}} \|f\|_{\mathcal{H}}$,
where $\mathcal{F} = \{f \in \mathcal{H} : f|_{E_1} = f_1\}$.

- **Sum** and **product** of RKs are still RKs.

- ◊ $K_1(x, y) + K_2(x', y')$: $\mathcal{H}_{K_1} \oplus \mathcal{H}_{K_2}$.

- ◊ $K_1(x, y) K_2(x', y')$: $\mathcal{H}_{K_1} \otimes \mathcal{H}_{K_2}$.

RKHS: Basics -5

- Discrete kernel **spectrum**.

- ◇ $K(x, y) = \sum_{j=1}^{\infty} \lambda_j \psi_j(x) \psi_j(y) =: \sum_{j=1}^{\infty} \tilde{\psi}_j(x) \tilde{\psi}_j(y),$

- ◇ where $\|\psi_j\|_{L_2(E, P)}^2 = 1$ and $\int K(x, y) \psi_j(y) dP(y) = \lambda_j \psi_j(x).$

- ◇ Note that, for $f(x) = \sum_j f_j \psi_j(x), \langle f, f \rangle_{\mathcal{H}} = \sum_j f_j^2 / \lambda_j.$

- ◇ $\{\tilde{\psi}_j = \sqrt{\lambda_j} \psi_j\}_{j=1}^{\infty}$: complete orthonormal basis for $\mathcal{H}.$

- If (E, P) is a finite measure space, then K has a discrete spectrum.

RKHS: Basics -6

Bounded linear functionals and operators on RKHS

- $\ell_f : \mathcal{H} \rightarrow \mathbb{R}$, $\ell_f(h) = \langle f, h \rangle_{\mathcal{H}}$ (Riesz representation).
- $\Sigma : \mathcal{H} \rightarrow \mathcal{H}$, there corresponds a kernel on $E \times E$ given by $\Sigma(x, t) = \Sigma K_x(t)$, where $K_x(t) =: K(x, t)$, as a function of t .

Kernel SVM (in brief)

SVM classification on RKHS

Training data: $\{x_i, y_i\}$, $x_i \in R^n$ and $y \in \{-1, 1\}$ for $i = 1, \dots, l$.

Goal: Look for a discriminant boundary, $f(x) = 0$, that separates the positive y 's from the negative y 's with "*maximum margin*".

Linear SVM: The algorithm looks for the separating hyperplane $w'x + b = 0$ with largest margin (given by $2/\|w\|_2$). That is, set $f(x) = w'x + b$, and solve the following constrained minimization problem:

$$\min_{w \in R^d} \frac{1}{2} \|w\|_2^2 + C \sum_{i=1}^l \xi_i \quad \text{subject to} \quad y_i f(x_i) \geq 1 - \xi_i, \quad \xi_i \geq 0, \quad \forall i = 1, \dots, l.$$

From linear SVM to kernel SVM

RKHS – a foundation for theoretical properties and
– a framework for efficient computation.

- start with a linear separation algorithm (maximizing margin)
- kernelization of the underlying linear learning algorithm,
- nonlinear separation \xrightarrow{RKHS} linear separation in feature space.
- sparse dual representation in an RKHS \rightarrow efficient algorithm,
- equivalence among regularization, sparse approximation, Bayesics, Gauss-Markov prediction (Huang and Lee, 2003);
likelihood-based statistical inference, etc.

SVM, linear separable case

$$\min_{w \in R^d, b \in R, \alpha_i \geq 0} \frac{1}{2} \|w\|_2^2 - \sum_{i=1}^l \alpha_i \{y_i (w' x_i + b) - 1\}.$$

$$\partial() / \partial b = 0 \rightarrow \sum_{i=1}^l \alpha_i y_i = 0$$

$$\partial() / \partial w = 0 \rightarrow w = \sum_{i=1}^l \alpha_i y_i x_i.$$

Dual problem:

$$\max_{\alpha_i \geq 0} \left(\sum_{i=1}^l \alpha_i - \frac{1}{2} \sum_{i,j=1}^l \alpha_i \alpha_j y_i y_j x_i' x_j \right) \text{ subject to } \sum_{i=1}^l \alpha_i y_i = 0.$$

SVM separating hyperplane:

$$f(x) = \sum_{i=1}^l \alpha_i y_i x_i' x + b,$$

with $b = -\frac{1}{2} \{ \max_{j \in I_-} (\sum_{i=1}^l \alpha_i y_i x_i' x_j) + \min_{j \in I_+} (\sum_{i=1}^l \alpha_i y_i x_i' x_j) \}$.

SVM, linear non-separable case

$$\min_{w \in R^d, b \in R, \xi_i \geq 0} \frac{1}{2} \|w\|_2^2 + C \sum_{i=1}^l \xi_i \quad \text{subject to} \quad y_i f(x_i) \geq 1 - \xi_i, \forall i = 1, \dots, l.$$

Dual problem:

$$\max_{0 \leq \alpha_i \leq C} \left(\sum_{i=1}^l \alpha_i - \frac{1}{2} \sum_{i,j=1}^l \alpha_i \alpha_j y_i y_j x_i' x_j \right) \quad \text{subject to} \quad \sum_{i=1}^l \alpha_i y_i = 0.$$

SVM separating hyperplane:

$$f(x) = \sum_{i=1}^l \alpha_i y_i x_i' x + b,$$

with $b = -\frac{1}{2} \{ \max_{j \in I_-^*} (\sum_{i=1}^l \alpha_i y_i x_i' x_j) + \min_{j \in I_+^*} (\sum_{i=1}^l \alpha_i y_i x_i' x_j) \}$,
where $*$: zero slack.

Kernel SVM

- Map the data in \mathcal{X} to some high dimensional space \mathcal{Z} , called the feature space: $x \rightarrow \tilde{\Psi}(x) = (\tilde{\psi}_1(x), \tilde{\psi}_2(x), \dots)'$,

- $K(x, u) = \sum_{\nu=1}^{\infty} \tilde{\psi}_{\nu}(x)\tilde{\psi}_{\nu}(u) = \sum_{\nu=1}^{\infty} \lambda_{\nu}\psi_{\nu}(x)\psi_{\nu}(u), \quad \lambda_{\nu} = \|\tilde{\psi}_{\nu}\|_2^2.$

$$f(x) = \sum_{\nu} f_{\nu}\psi_{\nu}(x), \quad \|f\|_{\mathcal{H}_K}^2 = \sum_{\nu} f_{\nu}^2/\lambda_{\nu}.$$

- feature mapping: $\mathcal{X} \rightarrow \mathcal{Z}$, linear separation on \mathcal{Z} .
RKs make the linear separation algorithm practically working without resorting to the feature mapping Ψ .

- SVM (a regularization problem on RKHS):

$$\min_{f \in \mathcal{H}_K + b} \frac{1}{2} \|f\|_{\mathcal{H}_K}^2 + C(\sum_{i=1}^l \xi_i)$$

$$\text{subject to } y_i f(x_i) \geq 1 - \xi_i, \quad \xi_i \geq 0, \quad \forall i = 1, \dots, l.$$

Kernel SVM, continued

Dual problem: $f(x) = \sum_{i=1}^l \alpha_i y_i K(x, x_i) + b$

$$\max_{0 \leq \alpha_i \leq C} \left(\sum_{i=1}^l \alpha_i - \frac{1}{2} \sum_{i,j=1}^l \alpha_i \alpha_j y_i y_j K(x_i, x_j) \right)$$

subject to $\sum_{i=1}^l \alpha_i y_i = 0.$

Two easy-to-understand kernels

$$\textit{linear spline} : K_{\text{lspl}}(t, s) = \min\{s, t\}, \quad s, t \in [0, 1],$$

$$\textit{Gaussian kernel} : K_{\text{rbf}}(t, s) = \exp\left\{-\frac{1}{2\sigma^2}\|t - s\|^2\right\}, \quad s, t \in R^d.$$

SVM with linear splines

◇ $K_{\text{Isb}}(t, s) = \min\{s, t\}$, $s, t \in [0, 1]$, is the reproducing kernel for the following RKHS:

$$\mathcal{H}_K = \{f : \text{abs. conti. on } [0, 1], f(0) = 0 \text{ and } \|f\|_{\mathcal{H}_K} = \|f'\|_2 < \infty\}.$$

◇ SVM: $\min_{f \in \mathcal{H}_K + b} \frac{1}{2} \|f\|_{\mathcal{H}_K}^2 + C \times (\text{data goodness of fit})$

subject to

◇ Regularize the first derivatives with penalty on $\|f'\|_2^2$.

SVM with Gaussian kernel

◇ $K_{\text{rbf}}(t, s) = \exp\left\{-\frac{1}{2\sigma^2}\|t - s\|^2\right\}$, $s, t \in \mathbb{R}^d$, is the reproducing kernel for the following RKHS:

$$\mathcal{H}_K = \left\{ f \in C^\infty : \|f\|_{\mathcal{H}_K}^2 = \sum_{k=0}^{\infty} \frac{\sigma^{2k}}{2^k k!} \|f^{(k)}\|_2^2 < \infty \right\}.$$

◇ SVM: $\min_{f \in \mathcal{H}_K + b} \frac{1}{2} \|f\|_{\mathcal{H}_K}^2 + C \times (\text{data goodness of fit})$

subject to

◇ Penalize on $\sum_{k=0}^{\infty} \frac{\sigma^{2k}}{2^k k!} \|f^{(k)}\|_2^2$.

Note the regularization on the k -th derivative is multiplied by σ^{2k} .

Kernel Fisher discriminant analysis

Classical Fisher linear discriminant analysis

- Input data: $\{x_j \in \mathcal{X} \subset \mathbb{R}^n\}_{j=1}^l$.
- Group labels: $\{y_j = \pm 1\}_{j=1}^l$.
- Find a discriminant hyperplane “ $w^t x + b = 0$ ”, which separates the two groups.

- Mahalanobis distance criterion: Classify a test input x by

$$\text{sign}\{d(x, \bar{x}_2) - d(x, \bar{x}_1)\},$$

where $d(x, \bar{x}_i) = (x - \bar{x}_i)^t S^{-1} (x - \bar{x}_i)$ with S the pooled covariance matrix. (i.e., $S = \sum_{i=1}^2 \sum_{j \in I_i} (x_j - \bar{x}_i)(x_j - \bar{x}_i)^t / l$.)

- Maximal likelihood ratio criterion: $x_j \sim N(\mu_i, \Sigma)$, $j \in I_i$. $\log MLR$

Kernel FDA – Ideas behind kernelization

- When the data space \mathcal{X} is not big enough for linear separation, or the coordinate system adopted is not feasible for linear separation, we resort to other means \rightarrow kernel approach.
- Map the data in \mathcal{X} to some high-dimensional Hilbert space (called the feature space) $\mathcal{Z} \subset R^q$. Often, $q = \infty$.

- Transformation:

$$z =: (\tilde{\psi}_1(x), \dots, \tilde{\psi}_q(x))^t =: (\sqrt{\lambda_1}\psi_1(x), \dots, \sqrt{\lambda_q}\psi_q(x))^t,$$

where $\{\psi_k\}_{k=1}^q$ are linear independent functions with unit L_2 -length, and $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_q > 0$.

- $K(x, u) =: z(x)^t z(u) = \sum_k \lambda_k \psi_k(x) \psi_k(u)$.

- Symbolically, “perform” the classical FLDA on the mapped data in \mathcal{Z} .

$$z \rightarrow \text{sign} \left\{ z^t S_w^{-1} (\bar{z}_1 - \bar{z}_2) - \frac{1}{2} (\bar{z}_1 + \bar{z}_2)^t S_w^{-1} (\bar{z}_1 - \bar{z}_2) \right\},$$

where $S_w = \sum_{j \in I} z_j z_j^t - \sum_{i=1}^2 l_i \bar{z}_i \bar{z}_i^t$.

- Since $S_w^{-1} (\bar{z}_1 - \bar{z}_2)$ is of form $\alpha_1 z_1 + \dots + \alpha_l z_l$,
the discriminant function is of form $f(x) = \sum_{j=1}^l \alpha_j K(x, x_j) + b$.
- Operate on $\{K(x_i, x_j)\}_{i,j=1}^l$ and group labels $\{y_j\}_{j=1}^l$. In practice, the kernel spectrum, given by Λ and Ψ , is not known.

Notation for KFDA

- Let I_1 be the index set of training sample for group label $y = 1$, I_2 for $y = -1$ and $I = I_1 \cup I_2$. Let $l_i = |I_i|$ be the size of I_i and $l = |I|$ be the size of I .
- Let $\mathbf{1} \in R^l$ be the vector of all ones, and let $\mathbf{1}_1, \mathbf{1}_2 \in R^l$ be as binary (0,1) vectors corresponding to their group label with 0 for non-members and 1 for members. With such definition, it leads to that $\mathbf{1}_1 + \mathbf{1}_2 = \mathbf{1}$.
- Let $Z =: (\Lambda^{1/2} \circ \Psi(x_1), \dots, \Lambda^{1/2} \circ \Psi(x_l))^t$, which is an $l \times n$ matrix. Let $K = ZZ^t$. Then, the (i, j) -th entry of K , denoted by K_{ij} , is given by $K(x_i, x_j)$.
- Let $\bar{z}_i = \frac{1}{l_i} \sum_{j \in I_i} z_j$, $i = 1, 2$, be the group centroid in the feature space, where $z_j(x) = \Lambda^{1/2} \circ \Psi(x_j)$, and let $\bar{z} = (\sum_{j=1}^l z_j)/l$.

- Let $\bar{k}_i = \frac{1}{l_i} \sum_{j \in I_i} K_j$, $i = 1, 2$, be the kernelized group centroid, where K_j is the j -th column vector of matrix K .
- Let $S_b = (\bar{z}_1 - \bar{z}_2)(\bar{z}_1 - \bar{z}_2)^t$ and $S_w = \sum_{j \in I} z_j z_j^t - \sum_{i=1}^2 l_i \bar{z}_i \bar{z}_i^t$ be the between- and within-class sample covariances for data in the feature space.
- Let $M_b = (\bar{k}_1 - \bar{k}_2)(\bar{k}_1 - \bar{k}_2)^t$ and $M_w = K^2 - \sum_{i=1}^2 l_i \bar{k}_i \bar{k}_i^t$ be the between- and within-class sample covariances for kernelized data.

KFDA in the feature space

Separating boundary : $z^t S_w^{-1}(\bar{z}_1 - \bar{z}_2) - \frac{1}{2}(\bar{z}_1 + \bar{z}_2)^t S_w^{-1}(\bar{z}_1 - \bar{z}_2) = 0$.

The KFDA finds the discriminant function of the form

$$f(x) = w^t z + b = \sum_{k=1}^d w_k \sqrt{\lambda_k} \psi_k(x) + b$$

passing through the mid point of group centroids, where w is the maximizing argument in the Rayleigh coefficient

$$J_{KFDA}(w) \equiv \frac{w^t S_b w}{w^t S_w w}.$$

A regularized within-class covariance of the form $S_w + rW$ is considered and w is the solution to the following maximization problem

$$\arg \max_{w \in R^q} J_{RKFDA}(w) \equiv \arg \max_{w \in R^q} \frac{w^t S_b w}{w^t (S_w + rW) w}.$$

The extra term rW is added to

- to overcome the numerical problem caused by singular within-class covariance in a high-dimensional feature space,
- to control the smoothness and the shape of the fitted discriminant hypersurface.

The discriminant function can be re-formulated as

$$f(x) = b + \sum_{j=1}^l \alpha_j K(x_j, x).$$

The coefficients α_j s can be obtained as the solution to the following maximization problem

$$\arg \max_{\alpha \in \mathbb{R}^l} J_{RKFDA}(\alpha) \equiv \arg \max_{\alpha \in \mathbb{R}^l} \frac{\alpha^t M_b \alpha}{\alpha^t (M_w + rA) \alpha}.$$

Again, the extra term rA is added to the within-class sample covariance for the same purposes as before.

In next slides we formulate the KFDA and its extension as a likelihood ratio of two Gaussians on an RKHS.

KFDA – a likelihood ratio criterion

- Classical FLDA: P_1 and P_2 Gaussian with a common covariance.

$$\log(dP_1(x)/dP_2(x)) = x^t \Sigma^{-1}(\mu_1 - \mu_2) - \frac{1}{2}(\mu_1 + \mu_2)^t \Sigma^{-1}(\mu_1 - \mu_2)$$

Plug in MLE for μ_i and Σ .

- Kernel FDA: Gaussian measures on RKHS, likelihood ratio, MLE.

Gaussian measure and covariance operator on an RKHS

Definition 1 (Gaussian measure on \mathcal{H}) A probability measure $P_{\mathcal{H}}$ on $(\mathcal{H}, \mathcal{T})$ is said to be Gaussian with respect to $\{\ell_f\}_{f \in \mathcal{H}}$ if for any k and any bounded linear functionals $\ell_{f_1}, \dots, \ell_{f_k}$ the joint distribution of $\ell_{f_1}(h), \dots, \ell_{f_k}(h)$ is normal, where h is a random element in \mathcal{H} with distribution $P_{\mathcal{H}}$.

Definition 2 (Covariance operator) A covariance operator, denoted by Σ , is defined to be an operator mapping from \mathcal{H} into \mathcal{H} which is bounded, linear, nonnegative definite, self-adjoint and trace class (i.e., of finite trace).

Let P_1 and P_2 be two equivalent probability measures on $(\mathcal{X}, \mathcal{B})$.

Consider the mapping $\gamma : x \rightarrow K(x, \cdot) =: K_x(\cdot) \in \mathcal{H}$. Let $P_{1, \mathcal{H}}$ and $P_{2, \mathcal{H}}$ denote the probability measures on $(\mathcal{H}, \mathcal{T})$ induced from P_1 and P_2 by γ . Assume that $P_{1, \mathcal{H}}$ and $P_{2, \mathcal{H}}$ are Gaussian with different mean functions

$$m_i(t) = E_{P_i} K_X(t) = \sum_{\nu} \lambda_{\nu} \psi_{\nu}(t) E_{P_i} \psi_{\nu}(X), \quad i = 1, 2,$$

and a common covariance operator

$$\Sigma_{\mathcal{H}}(s, t) = \text{cov}_{P_1}(K_X(s), K_X(t)) = \text{cov}_{P_2}(K_X(s), K_X(t)).$$

The mean functions and the covariance operator satisfy the following properties (see, for instance, Vakhania *et al.*, 1987)

$$E_{P_{i, \mathcal{H}}} \langle f, K_X \rangle_{\mathcal{H}} = \langle f, E_{P_i} K_X \rangle_{\mathcal{H}},$$

$$\text{cov}_{P_{i, \mathcal{H}}} \{ \langle f, K_X \rangle_{\mathcal{H}}, \langle g, K_X \rangle_{\mathcal{H}} \} = \langle \Sigma_{\mathcal{H}} f, g \rangle_{\mathcal{H}} = \langle f, \Sigma_{\mathcal{H}} g \rangle_{\mathcal{H}}.$$

Likelihood ratios

Theorem 1 (Grenander, 1952) *Let $P_{1,\mathcal{H}}$ and $P_{2,\mathcal{H}}$ be two equivalent Gaussian measures on $(\mathcal{H}, \mathcal{T})$ with mean $m_1(t)$ and $m_2(t)$ and a common covariance operator $\Sigma_{\mathcal{H}}$, which is assumed non-singular. Also assume that $(m_1 - m_2)$ is in the range of $\Sigma_{\mathcal{H}}$. Then the logarithm of the likelihood ratio is linear and given by*

$$\begin{aligned} & \log(dP_{1,\mathcal{H}}/dP_{2,\mathcal{H}})(K_x) \\ &= \langle K_x, \Sigma_{\mathcal{H}}^{-1}(m_1 - m_2) \rangle_{\mathcal{H}} - \frac{1}{2} \langle m_1 + m_2, \Sigma_{\mathcal{H}}^{-1}(m_1 - m_2) \rangle_{\mathcal{H}}, \end{aligned}$$

where $K_x(t) =: K(x, t)$, as a function of t .

- a test input $x \rightarrow$ a realization of the process $K_x(t)$,
- plug in MLE for means and covariance operator.

KFDA as a maximal likelihood ratio test

Classification for a test input x :

$$\begin{aligned} & \text{sign}\{\log(dP_{1,\mathcal{H}}/dP_{2,\mathcal{H}})(Kx)\} \\ &= \text{sign}\left\{\Sigma_{\mathcal{H}}^{-1}(m_1 - m_2)(x) - \frac{1}{2}\langle m_1 + m_2, \Sigma_{\mathcal{H}}^{-1}(m_1 - m_2)\rangle\right\}. \end{aligned}$$

Plug in ML estimates

$$\hat{m}_i(t) =: \frac{1}{l_i} \sum_{j \in I_i} K(x_j, t),$$

$$\hat{\Sigma}_{\mathcal{H}}(s, t) =: \frac{1}{l} \sum_{i=1}^2 \sum_{j \in I_i} (K(x_j, s) - \hat{m}_i(s))(K(x_j, t) - \hat{m}_i(t)) + \epsilon A(s, t).$$

With some technical details, then we result in the previously discussed KFDA algorithm.

Concluding remarks on kernelization

- Kernelization of a linear algorithm, or any convenient algorithm on \mathcal{X} leads to \longrightarrow same type of algorithm on an RKHS, but more flexible and versatile one on the original data space \mathcal{X} .
- RK provides a framework for efficient computation.
- RKHS lays a foundation for theory of statistical inference.

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The following is a list of selected references. Some short notes are appended based on the speaker's *subjective viewpoint* and *limited knowledge*.

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