Supervised learning
(VII) Support Vector Machine (SVM)

Séverine Affeldt

Université de Paris
Centre Borelli, CNRS

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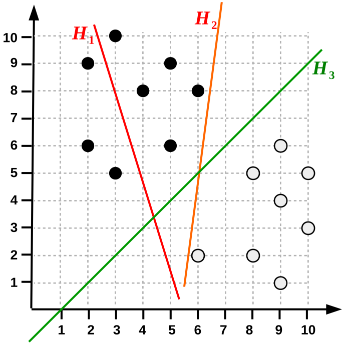
	x		
	x_1	x_2	y
i	1	9	-1
ii	2	6	-1
iii	2	8	-1
iv	3	10	-1
v	4	9	-1
vi	5	3	1
vii	5	8	-1
viii	5	10	-1
ix	6	2	1
x	6	5	1
xi	6	9	-1
xii	8	4	1
xiii	8	6	1
xiv	9	2	1
xv	9	5	1
xvii	10	3	1



Objective

Find the decision boundary that will indicate the class of a new *data point* **x** ?
- data point **x**: p−dimensional vector (eg. $\mathbf{x}_1 = (x_{1,1}, x_{1,2})$)
- decision boundary **H**: $(p-1)$−dimensional hyperplane (eg. $\mathbf{H_1}, \mathbf{H_2}, \mathbf{H_3}$)

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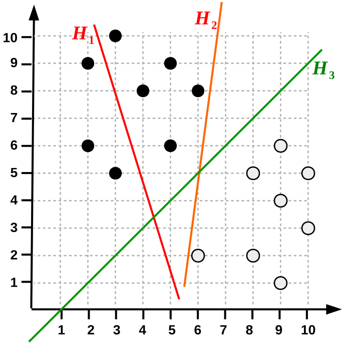

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SVM

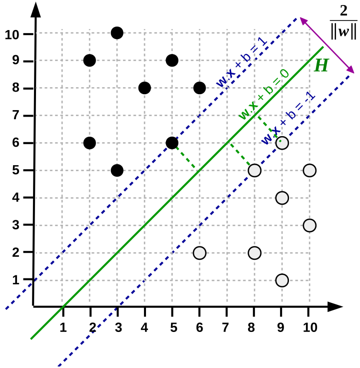
$\mathbf{H_3}$ is a reasonnable choice: maximises the **margin** between the two classes

(Vaplnik & Chervonenkis, 1963)

Decision boundary

Let us consider a training dataset of the form $\{(\mathbf{x_1}, y_1), (\mathbf{x_2}, y_2), ..., (\mathbf{x_n}, y_n)\}$, where $\mathbf{x_i}$ is a p dimensional **real** vector and $y_i \in \{-1, 1\}$. We want to find a hyperplane that maximizes the distance to the nearest $\mathbf{x_i}$.

Hyperplane H with parameters $\{w_i\}$ $\Leftrightarrow$ $\{\mathbf{x}\}, \quad \sum_{i=1}^{n} w_i x_i + b = \langle \mathbf{w}.\mathbf{x} \rangle + b = 0$

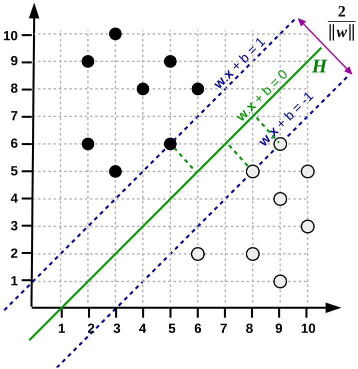


Linearly separable data

∃ **two parallel** hyperplanes that separate the data, such that the **distance** between them is as **large** as possible. This distance is the **margin**.

(1) $\langle \mathbf{w}.\mathbf{x} \rangle + b = 1$
(2) $\langle \mathbf{w}.\mathbf{x} \rangle + b = -1$

Where does the **margin** come from?



Objective

Maximizing the margin $\Leftrightarrow$ find $\mathbf{w}$ s.t. $max(\frac{2}{\|\mathbf{w}\|}) \Leftrightarrow$ find $\mathbf{w}$ s.t. $min(\|\mathbf{w}\|)$, $\|\mathbf{w}\|=\sqrt{w_1^2+w_2^2+\ldots}$

Supplementary constraint

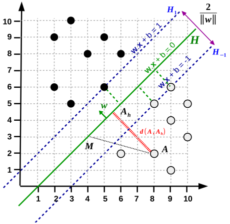
No data point within the margin!

$\forall i$,

$\langle \mathbf{w}.\mathbf{x}^{s_i} \rangle + b \geq 1$, *if* $y_i = 1$

or

$\langle \mathbf{w}.\mathbf{x}^{s_i} \rangle + b \leq -1$, *if* $y_i = -1$



All in all,

$\forall\ 1 \leq i \leq\ n,\ \ y_i(\langle \mathbf{w}.\mathbf{x}^{s_i} \rangle + b) \geq 1$

Full SVM objective

Minimizing $\|\mathbf{w}\|$, where $\|\mathbf{w}\|=\sqrt{w_1^2+w_2^2+\ldots}$, and subject to $y_i(\langle \mathbf{w}.\mathbf{x}^{s_i} \rangle + b) \geq 1,\ \forall\ 1 \leq i \leq\ n$

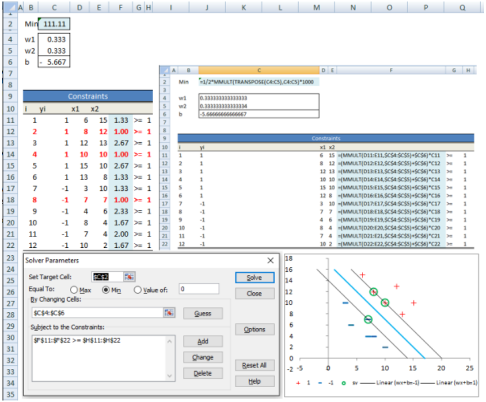
Our classifier is defined by $\mathbf{w}$ and b that satisfy this requirements. It is **fully** determined by the closest samples $\mathbf{x}^{s_i}$, which are named **support vectors**.

Primal form of the optimization problem

$$\text{Minimizing } \frac{1}{2}(w_1^2+w_2^2+\ldots+w_p^2) \quad \text{subject to} \quad y_i(\langle \mathbf{w}.\mathbf{x}^{s_i}\rangle+b) \geq 1,\ \forall\ 1\leq i\leq\ n$$

$\Rightarrow$ a well known quadratic optimization problem, where we have a **quadratic objective** function subject to **linear constraints**.
$\Rightarrow$ not possible for large p ($>$ few hundreds)...
$\Rightarrow$ not applicable to non linearly separable data...

Toy example with the Excel Solver(12 constraints)



Dual form of the optimization problem

Minimizing $\frac{1}{2}(w_1^2+w_2^2+\ldots+w_p^2)$ subject to $y_i(\langle \mathbf{w}.\mathbf{x}^{s_i}\rangle+b) \geq 1,\ \forall\ 1\leq i\leq\ n$

Set up a **Lagrange** function and derive the solution **analytically**

[1] Karush, Kuhn & Tucker

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Set up a **Lagrange** function and derive the solution **analytically**

Rewrite the constraint,

$y_i(\langle \mathbf{w}.\mathbf{x}^{s_i}\rangle + b) - 1 \ \geq \ 0$

Multiple by Lagrange multipliers (α_i) and subtract from the objective function,

$argmin_{\mathbf{w},b} \ \ L(\mathbf{w}, b, \alpha) = \frac{1}{2}\langle \mathbf{w}^{\mathbf{T}}.\mathbf{w}\rangle - \sum_{i=1}^{n} \alpha_i(y_i(\langle \mathbf{w}.\mathbf{x}^{s_i}\rangle + b) - 1)$, where $\alpha_i \geq 0$

NB: minimizing with respect to $\mathbf{w}$ *and b...but maximizing with respect to* $\{\alpha_i\}$

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NB: minimizing with respect to **w** *and b...but maximizing with respect to* $\{\alpha_i\}$

A quadratic optimization problem **must** satisfied the KKT[1] conditions,

(1) $\nabla_{\mathbf{w}} L(\mathbf{w}, b, \alpha) = 0$ & $\frac{\partial L(\mathbf{w},b,\alpha)}{\partial b} = 0$

(2) $\alpha_i \geq 0$

(3) $\alpha_i(y_i(\langle \mathbf{w}.\mathbf{x}^{s_i}\rangle + b) - 1) \ = \ 0$

(4) $y_i(\langle \mathbf{w}.\mathbf{x}^{s_i}\rangle + b) - 1 \ \geq \ 0$

Caution: $\alpha_i > 0 \Rightarrow x_i$ is a $\boxed{\text{support vector}}$

[1] Karush, Kuhn & Tucker

Conditions

$$L(\mathbf{w},b,\alpha)=\frac{1}{2}\langle \mathbf{w}.\mathbf{w}\rangle-\sum_{i=1}^{n}\alpha_i(y_i(\langle \mathbf{w}.\mathbf{x}^{s_i}\rangle+b)-1)$$

(1) $\nabla_{\mathbf{w}}L(\mathbf{w},b,\alpha)=0$ & $\frac{\partial L(\mathbf{w},b,\alpha)}{\partial b}=0$

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(3) $\alpha_i(y_i(\langle \mathbf{w}.\mathbf{x}^{s_i}\rangle+b)-1)=0$

(4) $y_i(\langle \mathbf{w}.\mathbf{x}^{s_i}\rangle+b)-1\geq 0$

Lagrangian expansion

$$L(\mathbf{w},b,\alpha)=\frac{1}{2}\langle \mathbf{w}.\mathbf{w}\rangle-\sum_{i=1}^{n}\alpha_i(y_i\langle \mathbf{w}.\mathbf{x}^{s_i}\rangle+y_ib-1)$$

$$L(\mathbf{w},b,\alpha)=\frac{1}{2}\langle \mathbf{w}.\mathbf{w}\rangle-\sum_{i=1}^{n}\alpha_iy_i\langle \mathbf{w}.\mathbf{x}^{s_i}\rangle+\sum_{i=1}^{n}\alpha_iy_ib-\sum_{i=1}^{n}\alpha_i$$

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Getting the dual formulation

(1) $\nabla_{\mathbf{w}} = \mathbf{w}-\sum_{i=1}^{n}\alpha_iy_i\mathbf{x}^{s_i} \Rightarrow \boxed{\mathbf{w} = \sum_{i=1}^{n}\alpha_iy_i\mathbf{x}^{s_i}}$

(2) $\frac{\partial L(\mathbf{w},b,\alpha)}{\partial b} = -\sum_{i=1}^{n}\alpha_iy_i \Rightarrow \boxed{-\sum_{i=1}^{n}\alpha_iy_i = 0}$

...substituting in expanded Lagrangian...

$$\boxed{L(\alpha) = \sum_{i=1}^{n}\alpha_i-\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_jy_iy_j\langle\mathbf{x}^{s_i}\mathbf{x}^{s_j}\rangle}$$

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Dual formulation of the optimization problem

$$argmax_\alpha \; L(\alpha) = \sum_{i=1}^{n}\alpha_i-\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_jy_iy_j\langle\mathbf{x}^{s_i}\mathbf{x}^{s_j}\rangle, \quad \text{where} \quad \alpha_i\geq 0 \;\&\; \sum_{i=1}^{n}\alpha_iy_i = 0$$

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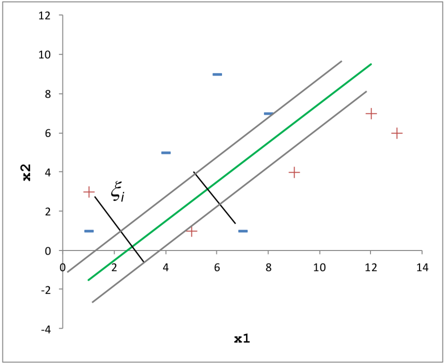
NB: Instead of minimizing over $\mathbf{w}$ and b subject to linear constraints, we can maximize over α

In practice, there is no perfect separation!



- ξ est un vecteur de taille n
- $\xi_i \geq 0$ matérialise l'erreur de classement pour chaque observation
- $\xi_i = 0$, elle est nulle lorsque l'observation est du bon côté de la droite « marge » associée à sa classe
- $\xi_i < 1$, le point est du bon côté de la frontière, mais déborde de la droite « marge » associée à sa classe
- $\xi_i > 1$, l'individu est mal classé

In practice, there is no perfect separation!

Formulation primale

$$\min_{\beta,\beta_0,\xi_i} \frac{1}{2}\|\beta\|^2 + C\sum_{i=1}^{n}\xi_i$$

$s.c.$

$$y_i \times (x_i^T\beta + \beta_0) \geq 1 - \xi_i, \forall i = 1,\ldots,n$$

$$\xi_i \geq 0, \ \forall i$$

Formulation duale

$$\max_{\alpha} L_D(\alpha) = \sum_{i=1}^{n}\alpha_i - \frac{1}{2}\sum_{i=1}^{n}\sum_{i'=1}^{n}\alpha_i\alpha_{i'}y_i y_{i'}\langle x_i, x_{i'}\rangle$$

$s.c.$

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

$$0 \leq \alpha_i \leq C, \ \forall i$$

La tolérance aux erreurs est plus ou moins accentuée avec le paramètre **C** (''cost'' parameter)

➔ C trop élevé, danger de sur-apprentissage

➔ C trop faible, sous-apprentissage

In practice, there is no perfect separation!

'Soft' Primal formulation

$$argmin_{\mathbf{w},b,\xi^{s_i}} \ \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{n}\xi_i, \quad \xi^{s_i} \text{ tolerance or classification error, } C \text{ cost}$$

with constraints,

$$\forall\ i,\ 1 \ \leq \ i \ \leq \ n, \quad y_i(\langle \mathbf{w}.\mathbf{x}^{S_i}\rangle + b) \geq 1 - \xi^{s_i} \qquad \& \qquad \xi^{S_i} \geq 0$$

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$$argmax_{\alpha} \ L(\alpha) \ = \ \sum_{i=1}^{n}\alpha_i - \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j y_i y_j \langle \mathbf{x}^{s_i}\mathbf{x}^{s_j}\rangle$$

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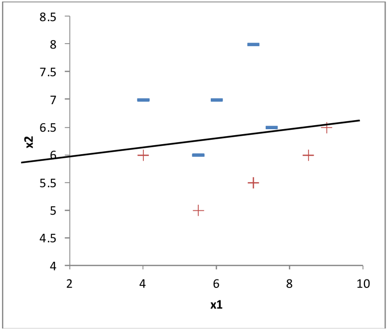
$$\forall\ i,\ 1 \ \leq \ i \ \leq \ n, \quad 0 \leq \alpha_i \leq C \qquad \& \qquad \sum_{i=1}^{n}\alpha_i y_i \ = \ 0$$

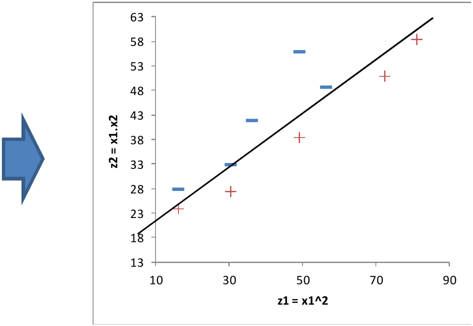
About the cost ξ^{s_i} and C

OK $\Rightarrow \xi^{s_i} = 0$; OK but within margin $\Rightarrow \xi^{s_i} < 1$; not OK $\Rightarrow \xi^{s_i} > 1$

C too high $\Rightarrow$ overfitting; C too low $\Rightarrow$ underfitting

With *appropriate* variable transformations, we can turn a non linearly separable problem into a linearly separable one!
An example: $\Phi(\mathbf{x} = (x_1, x_2)) = (x_1^2, x_1 x_2)$





Dual formulation of the optimization problem

$$argmax_{\alpha} \;\; L(\alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \langle \mathbf{x}^{s_i} \mathbf{x}^{s_j} \rangle, \quad \text{where} \quad \alpha_i \geq 0 \;\&\; \sum_{i=1}^{n} \alpha_i y_i = 0$$

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Directly transforming the variables

An example: $\Phi(\mathbf{x} = (x_1, x_2)) = (x_1^2, \sqrt(2) x_1 x_2, x_2^2)$
We need to compute all the $\langle \Phi(\mathbf{x}^{\mathbf{s_i}}) \Phi(\mathbf{x}^{\mathbf{s_j}}) \rangle$, and we need to manipule 3 variables instead of 2... This is time and memory costly...

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Using a Kernel function

$K(\mathbf{x}^{s_i}, \mathbf{x}^{s_j}) = \langle \Phi(\mathbf{x}^{s_i}), \Phi(\mathbf{x}^{s_j})\rangle$
Here, we compute the scalar product (as before), and convert only the result with K!
We manipulate only 2 variables, but still, we are in a higher dimension.

Dual formulation of the optimization problem

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Let us consider two data points/vectors,
$\mathbf{u} = (4, 7)$ & $\mathbf{v} = (2, 5) \Rightarrow \langle \mathbf{u}, \mathbf{v} \rangle = 4 \times 2 + 5 \times 7 = 43$

Example (a)

$\Phi(\mathbf{x} = (x_1, x_2)) = (x_1^2, \sqrt{2} x_1 x_2, x_2^2)$
$\Phi(\mathbf{u} = (16, 39.6, 49))$ & $\Phi(\mathbf{v} = (4, 14.1, 25))$
$\Rightarrow \langle \Phi(\mathbf{u}), \Phi(\mathbf{v}) \rangle = 1849$

<u>Using the corresponding K</u>, $K_1(\mathbf{u}, \mathbf{v}) = (\langle \mathbf{u}, \mathbf{v} \rangle)^2 = 43^2 = 1849$

Dual formulation of the optimization problem

$$argmax_{\alpha}\ L(\alpha) = \sum_{i=1}^{n}\alpha_i - \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j y_i y_j \langle \mathbf{x}^{s_i}\mathbf{x}^{s_j}\rangle, \quad \text{where} \quad \alpha_i \geq 0 \ \& \ \sum_{i=1}^{n}\alpha_i y_i = 0$$

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Using the corresponding K, $K_1(\mathbf{u}, \mathbf{v}) = (\langle \mathbf{u}, \mathbf{v}\rangle)^2 = 43^2 = 1849$

Example (b)

$\Phi(\mathbf{x} = (x_1, x_2)) = (1, \sqrt{2}x_1, \sqrt{2}x_2, x_1^2, x_2^2, \sqrt{2}x_1x_2, x_2^2)$
$\Phi(\mathbf{u} = (1, 5.7, 9.9, 16, 49, 39; 6))$ & $\Phi(\mathbf{v} = (1, 2.8, 7.1, 4, 25, 14.1))$
$\Rightarrow \langle \Phi(\mathbf{u}), \Phi(\mathbf{v})\rangle = 1936$

Using the corresponding K, $K_2(\mathbf{u}, \mathbf{v}) = (1 + \langle \mathbf{u}, \mathbf{v}\rangle)^2 = (1 + 43)^2 = 1936$

With a kernel function K, computations are equivalent, but we project all data points into a higher dimensional space without explicitly transforming the data points.

'Soft' Dual formulation of the optimization problem with a kernel function

$$argmax_{\alpha} \; L(\alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j K(\mathbf{x}^{s_i} \mathbf{x}^{s_j}), \quad \text{where} \quad 0 \leq \alpha_i \leq C \;\&\; \sum_{i=1}^{n} \alpha_i y_i = 0$$

Classification with a kernel function

$$\boxed{f(x_i) = \sum_{i \in SV} \alpha_i y_i K(\mathbf{x_i}.\mathbf{x}) + b}$$

Polynomial Kernel

$$K(\mathbf{u}, \mathbf{v}) = (coef0 + \langle \mathbf{u}, \mathbf{v} \rangle)$$

Radial basis Kernel

$$K(\mathbf{u}, \mathbf{v}) = exp(-\gamma \times \|\mathbf{u} - \mathbf{v}\|^2)$$

Sigmoid Kernel

$$K(\mathbf{u}, \mathbf{v}) = tanh(-\gamma \times \langle \mathbf{u}, \mathbf{v} \rangle + coef0)$$

NB: More kernel functions in LIBSVM, available in `scikit-learn` or `e1071`

Bibliography

- Ng, Andrew. "CS 229 Lecture Notes: Support Vector Machines.", cs229.stanford.edu/notes (2012)
- Rakotomalala, Ricco. "Machines à Vecteurs de Support."

A reminder on normal vector and direction vector

Normal vector

If (d) is a line defined by the equation $ax + by + c = 0$, then $v = (a, b)$ is a vector normal to (d).

Let's choose two points, $A = (x_A, y_A)$ and $M = (x, y)$ that belong to (d). If v is normal to (d), then $< AM.v > = < (x_A - x, y_A - y).(a, b) > = 0$.

Hence, A and M are such that $a(x - x_A) + b(y - y_A) = 0 \Leftrightarrow ax + by + c = 0$, with $c = -(ax_A + by_A)$

Direction vector

A direction vector of (d) is $u = (-b, a)$.

Distance $d(A, A_h)$

$\mathbf{w}=(w_1, w_2)^T$ is a vector **normal** to H.

$\forall M \in H, \quad \langle \mathbf{AM}.\mathbf{w}\rangle = \langle (\mathbf{AA_h}+\mathbf{A_hM}).\mathbf{w}\rangle = \langle \mathbf{AA_h}.\mathbf{w}\rangle$

$$\langle \mathbf{AA_h}.\mathbf{w}\rangle = w_1(x_{A_h}-x_A)+w_2(y_{A_h}-y_A)$$
$$\langle \mathbf{AA_h}.\mathbf{w}\rangle = w_1 x_{A_h}+w_2 y_{A_h}-w_1 x_A - w_2 y_A$$
$$\langle \mathbf{AA_h}.\mathbf{w}\rangle = -w_1 x_A - w_2 y_A - b \qquad (A_h \in H)$$

...and...

$$\langle \mathbf{AA_h}.\mathbf{w}\rangle = \|\mathbf{AA_h}\|\,\|\mathbf{w}\|$$

$$\Rightarrow d(A, A_h) = \|\mathbf{AA_h}\| = \frac{|w_1 x_A + w_2 y_A + b|}{\|\mathbf{w}\|}$$

If $A \in H_1$ or $A \in H_{-1}$, $\|\mathbf{AA_h}\| = \frac{1}{\|\mathbf{w}\|}$

...hence...

$$\boxed{Margin = \frac{2}{\|\mathbf{w}\|}}$$