annotated version

Machine Learning Course - CS-433

Cost Functions

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minor changes by Martin Jaggi 2016

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ÉCOLE POLYTECHNIQUE
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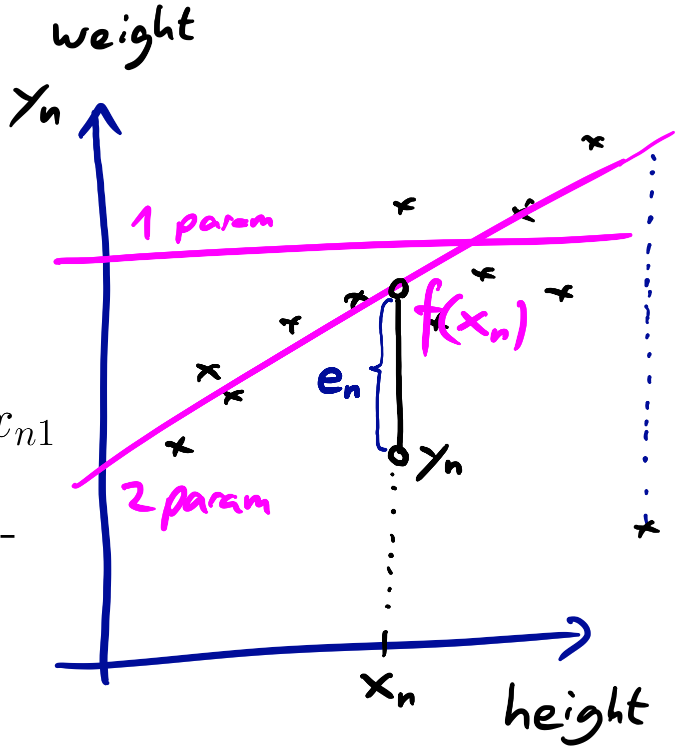
Motivation

Consider the following models.

1-parameter model: $y_n \approx w_0$
2-parameter model: $y_n \approx w_0 + w_1 x_{n1}$

How can we estimate (or guess) values of $\mathbf{w}$ given the data $\mathcal{D}$?



What is a cost function?

A cost function (or energy, loss, training objective) is used to learn parameters that explain the data well. The cost function quantifies how well our model does - or in other words how costly our mistakes are.

Two desirable properties of cost functions

When the target y is real-valued, it is often desirable that the cost is symmetric around 0, since both positive and negative errors should be penalized equally.

Also, our cost function should penalize "large" mistakes and "very-large" mistakes similarly.

Robustness

Statistical vs computational trade-off

If we want better statistical properties, then we have to give-up good computational properties.

Robustness

Efficient Training (see later)

Mean Square Error (MSE)

MSE is one of the most popular cost functions.

$$\mathrm{MSE}(\mathbf{w}) := \frac{1}{N}\sum_{n=1}^{N} \underbrace{\left[\overbrace{y_n - f(\mathbf{x}_n)}^{e_n}\right]^2}_{\text{error of n-th datapoint}}$$

Does this cost function have both mentioned properties?

An exercise for MSE

Compute MSE for 1-param model:

$$f(x_n) = f_w(x_n)$$

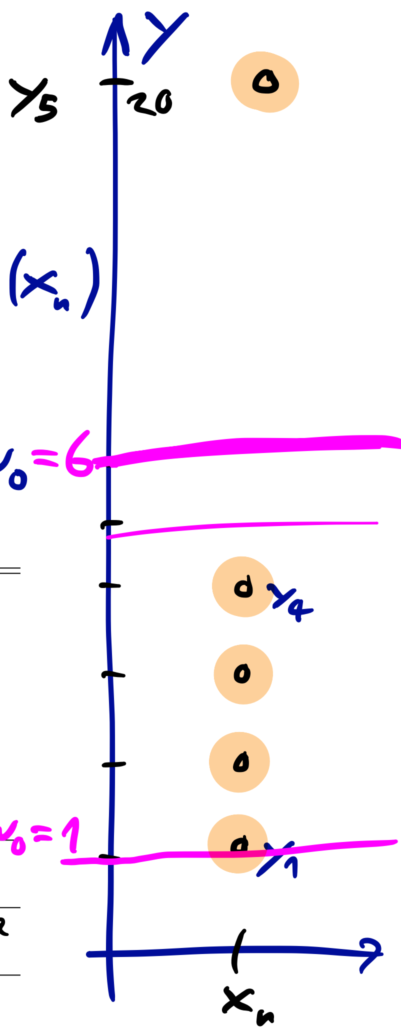
$$\mathcal{L}(w_0) := \frac{1}{N}\sum_{n=1}^{N} [\underbrace{y_n - w_0}_{e_n}]^2$$

w_0

$N=5$

	1	2	3	4	5	6	7
$y_1 = 1$	0	1	2^2	3^2	4^2	5^2	6^2
$y_2 = 2$	1	0	1	2^2	3^2	4^2	5^2
$y_3 = 3$	4	1	0	1	2^2	3^2	4^2
$y_4 = 4$	9	2^2	1	0	1	2^2	3^2
$\mathrm{MSE}(\mathbf{w}) \cdot N$	14	6	6	14	30	54	
$y_5 = 20$	19^2	18^2	17^2	16^2	15^2	14^2	13^2
$\mathrm{MSE}(\mathbf{w}) \cdot N$	...	..	..			250	

Some help: $19^2 = 361, 18^2 = 324, 17^2 = 289, 16^2 = 256, 15^2 = 225, 14^2 = 196, 13^2 = 169$.



best model $w_0=2,3$

best $w_0=6$

Outliers

Outliers are data examples that are far away from most of the other examples. Unfortunately, they occur more often in reality than you would want them to!

data-point (x_s, y_s)

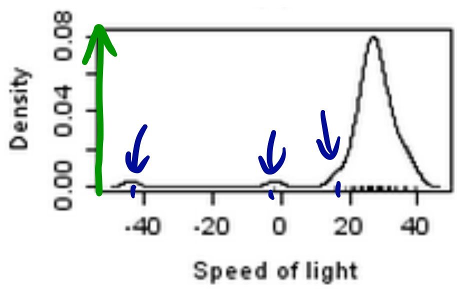
MSE is not a good cost function when outliers are present.

not robust

Here is a real example on speed of light measurements (Gelman's book on Bayesian data analysis)

28	26	33	24	34	-44	27	16	40	-2
29	22	24	21	25	30	23	29	31	19
24	20	36	32	36	28	25	21	28	29
37	25	28	26	30	32	36	26	30	22
36	23	27	27	28	27	31	27	26	33
26	32	32	24	39	28	24	25	32	25
29	27	28	29	16	23				

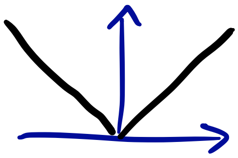
(a) Original speed of light data done by Simon Newcomb.



(b) Histogram showing outliers.

Handling outliers well is a desired *statistical* property.

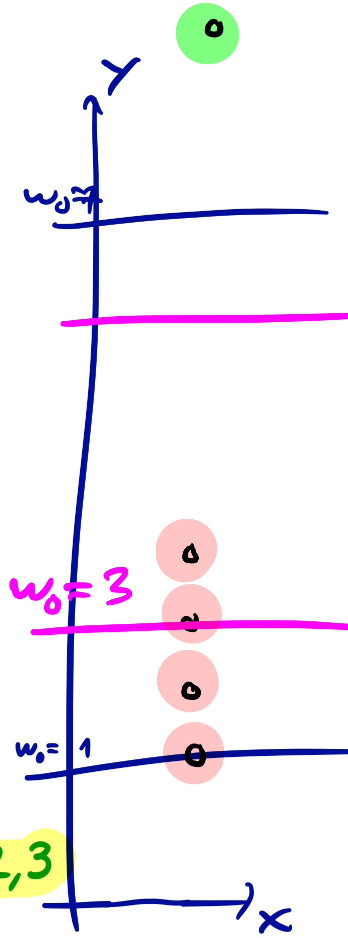
Mean Absolute Error (MAE)



$$\mathrm{MAE}(\mathbf{w}) := \frac{1}{N}\sum_{n=1}^{N} \left|\overbrace{y_n - f(\mathbf{x}_n)}^{e_n}\right|$$

robust

Repeat the exercise with MAE.

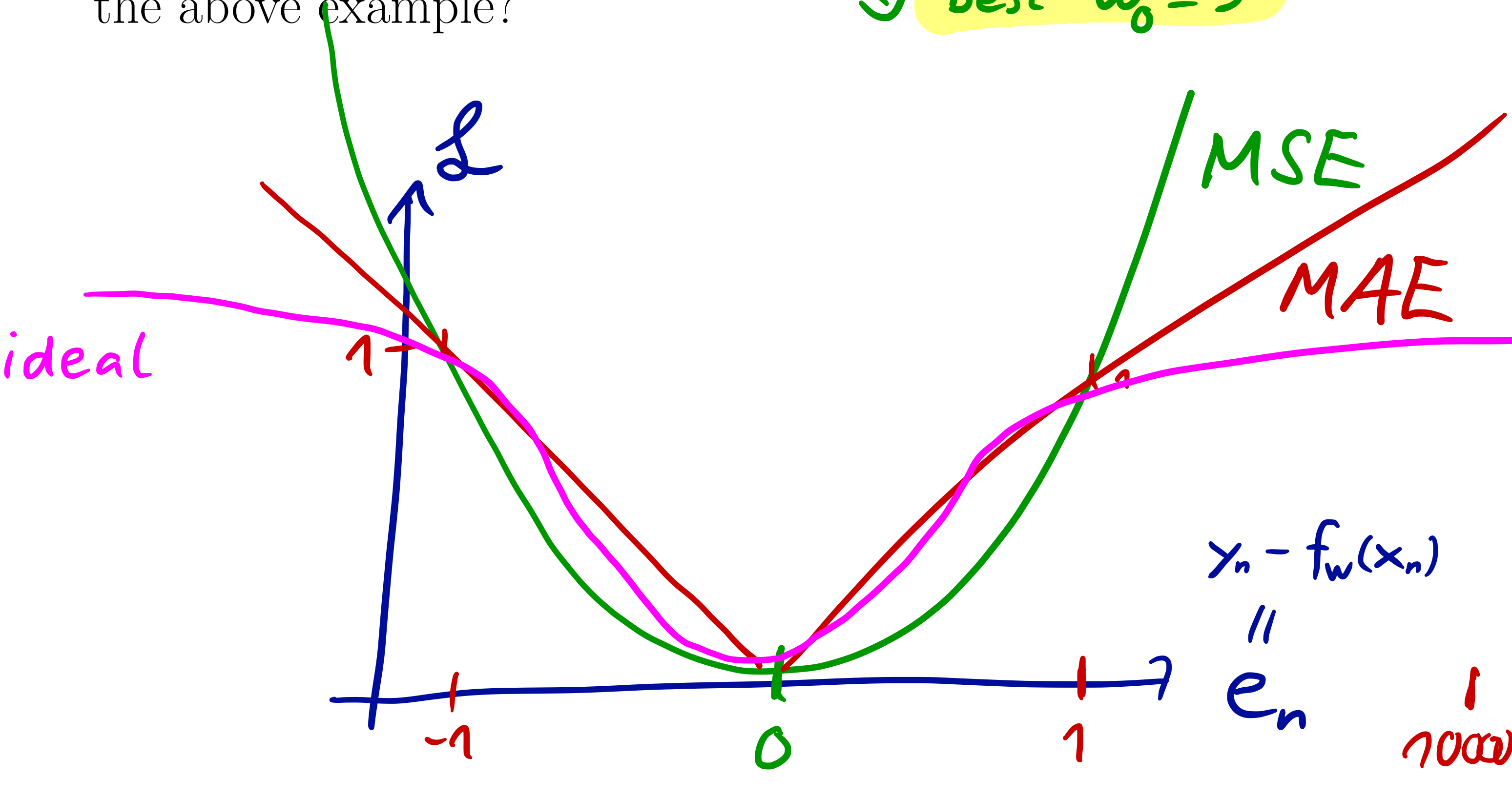


	$w_0=$ 1	2	3	4	5	6	$w_0=$ 7
$y_1 = 1$	0	1	2	3	4	5	6
$y_2 = 2$	1	0	1	2	3	4	5
$y_3 = 3$	2	1	0	1	2	3	4
$y_4 = 4$	3	2	1	0	1	2	3
$\mathrm{MAE}(\mathbf{w}) \cdot N$	6	4	4	6	10	14	18
$y_5 = 20$	19	18	17	16	15	14	13
$\mathrm{MAE}(\mathbf{w}) \cdot N$	25	22	21	22	25		

best $w_0 = 2,3$

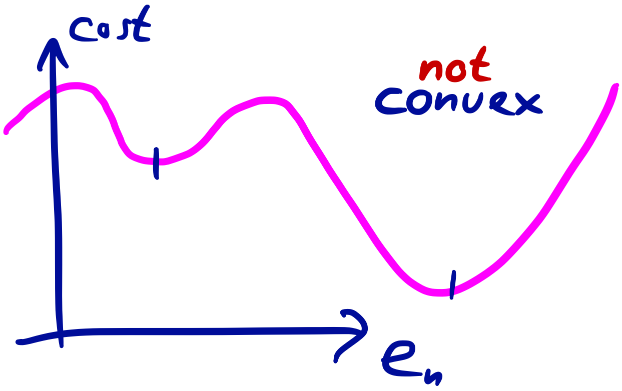
best $w_0 = 3$

Can you draw MSE and MAE for the above example?



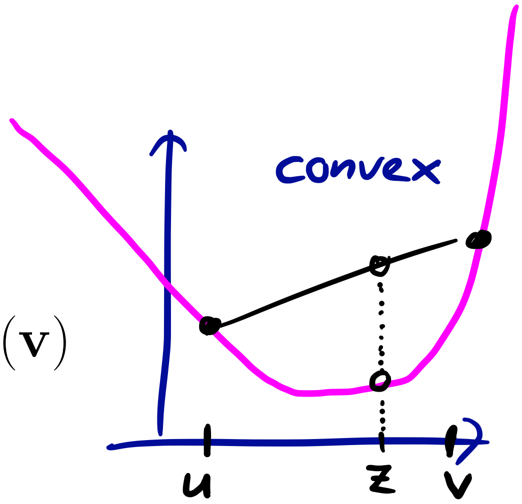
Convexity

Roughly, a function is convex iff a line joining two points never intersects with the function anywhere else.



A function $f(\mathbf{u})$ with $\mathbf{u} \in \mathcal{X}$ is convex, if for any $\mathbf{u}, \mathbf{v} \in \mathcal{X}$ and for any $0 \leq \lambda \leq 1$, we have:

$$f(\underbrace{\lambda \mathbf{u} + (1-\lambda)\mathbf{v}}_{z}) \leq \lambda f(\mathbf{u}) + (1-\lambda) f(\mathbf{v})$$



A function is strictly convex if the inequality is strict. <

Importance of convexity

A strictly convex function has a unique global minimum $\mathbf{w}^\star$. For convex functions, every local minimum is a global minimum.

$$\mathcal{L}\big(\underbrace{y_n - (f_w(x) = w^T x)}_{e_n}\big)$$

Sums of convex functions are also convex. Therefore, MSE is convex.

as a function of e_n.

Convexity is a desired *computational* property.

Same for MAE

Can you prove that the MAE is convex? (as a function of the parameters $\mathbf{w} \in \mathbb{R}^D$, for linear regression $f(\mathbf{x}) := \mathbf{x}^\top \mathbf{w}$)

Homework!

Computational VS statistical trade-off

So which loss function is the best?

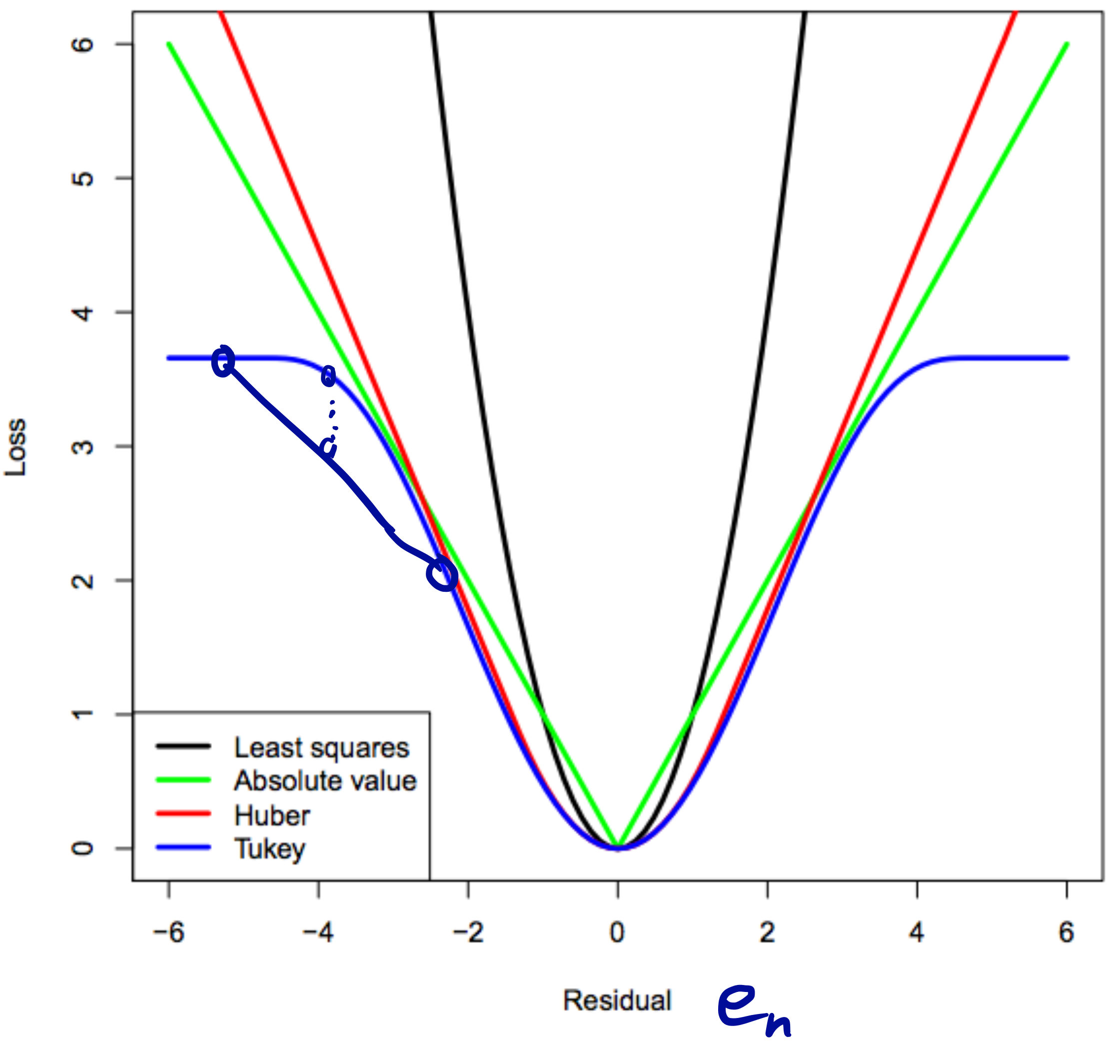


Figure taken from Patrick Breheny's slides.

If we want better statistical properties, then we have to give-up good computational properties.

Additional Reading

Other cost functions

Huber loss

$$Huber := \begin{cases} \frac{1}{2}e^2 & \text{, if } |e| \leq \delta \\ \delta|e| - \frac{1}{2}\delta^2 & \text{, if } |e| > \delta \end{cases} \tag{1}$$

Huber loss is convex, differentiable, and also robust to outliers. However, setting δ is not an easy task.

Tukey's bisquare loss (defined in terms of the gradient)

$$\frac{\partial \mathcal{L}}{\partial e} := \begin{cases} e\{1 - e^2/\delta^2\}^2 & \text{, if } |e| \leq \delta \\ 0 & \text{, if } |e| > \delta \end{cases} \tag{2}$$

Tukey's loss is non-convex, but robust to outliers.

Additional reading on outliers

- Wikipedia page on "Robust statistics".
- Repeat the exercise with MAE.
- Sec 2.4 of Kevin Murphy's book for an example of robust modeling

Nasty cost functions: Visualization

See Andrej Karpathy Tumblr post for many cost functions gone "wrong" for neural networks. `http://lossfunctions.tumblr.com/`.