EEN1083

Data analysis and machine learning I

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Regularization

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Outline

Norms

Overfitting

Regularization

L2 regularization

L1 regularization

Norms

In mathematics, a norm is a function from a real or complex vector space to the non-negative real numbers that behaves in certain ways like the distance from the origin: it commutes with scaling, obeys a form of the triangle inequality, and is zero only at the origin. (Wikipedia)

In machine learning norms are a way to measure the size of a vector, matrix or tensor

Norms

Most common norm is the Euclidean norm or L_2 norm, denoted $\|\mathbf{x}\|_2$ or just $\|\mathbf{x}\|$. Gives the length of the vector.

$$\|\mathbf{x}\| = \sqrt{\mathbf{x}^T\mathbf{x}} = \sqrt{\sum_i x_i^2}$$

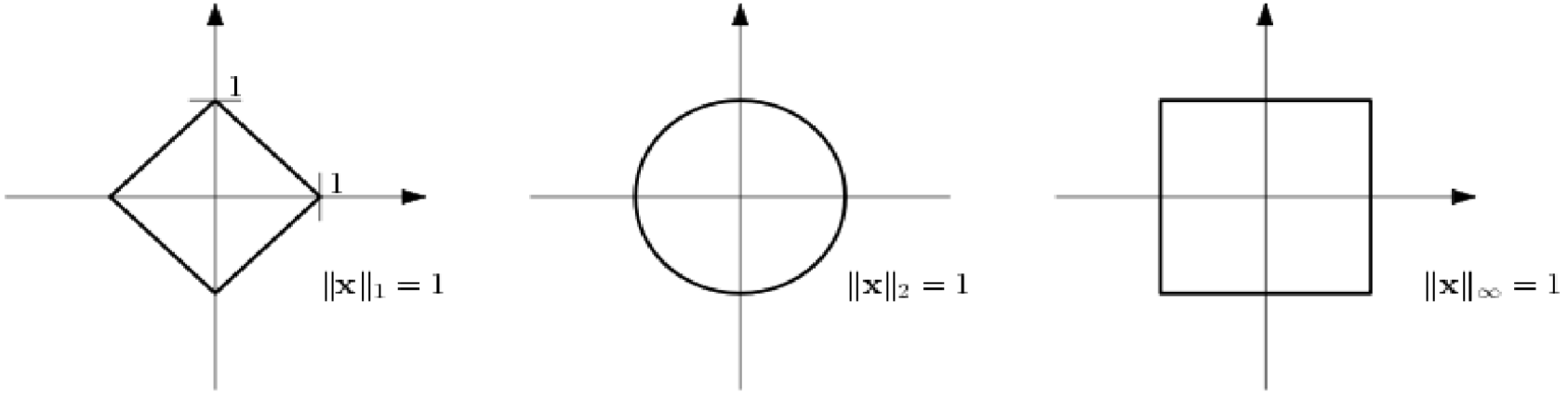
The squared Euclidean norm $\|\mathbf{x}\|_2^2$ is often useful:

$$\|\mathbf{x}\|^2 = \mathbf{x}^T\mathbf{x} = \mathbf{x} \cdot \mathbf{x}$$

Another common norm is the L_1 norm, which is the sum of absolute values of $\mathbf{x}$

$$\|\mathbf{x}\|_1 = \sum_i |x_i|$$

Norms



Properties of norms

A norm is any function p from vectors to $\mathbb{R}$ that satisfies:

1. $p(\alpha \mathbf{x}) = |\alpha| p(\mathbf{x})$ for $\alpha \in \mathbb{R}$
2. $p(\mathbf{x} + \mathbf{y}) \leq p(\mathbf{x}) + p(\mathbf{y})$ (triangle inequality)
3. $p(\mathbf{x}) = 0 \iff \mathbf{x} = \mathbf{0}$

E.g. $\|5\mathbf{x}\| = 5\|\mathbf{x}\|$ for any norm $\|\cdot\|$.
We also have $p(-\mathbf{x}) = p(\mathbf{x})$

Norms and distance metrics

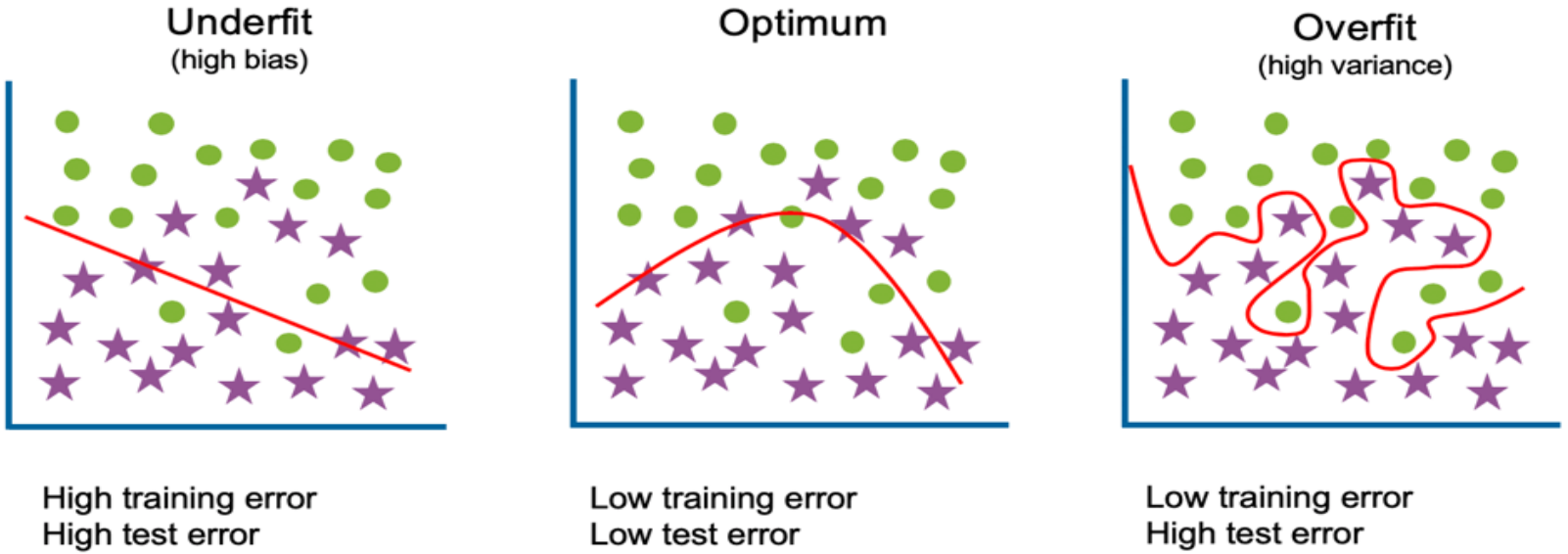
Any vector space V and norm p can be used to induce a distance metric (define a **metric space**) by defining the distance metric to be $d(\mathbf{x}, \mathbf{y}) = p(\mathbf{x} - \mathbf{y})$

E.g. The space of D dimensional real valued vectors $\mathbb{R}^D$ and the L_2 norm give the Euclidean space with metric $d(\mathbf{x}, \mathbf{y}) = \|\mathbf{x} - \mathbf{y}\|_2$.

In 2D this gives the familiar Euclidean distance between two points $\mathbf{x}$ and $\mathbf{y}$:

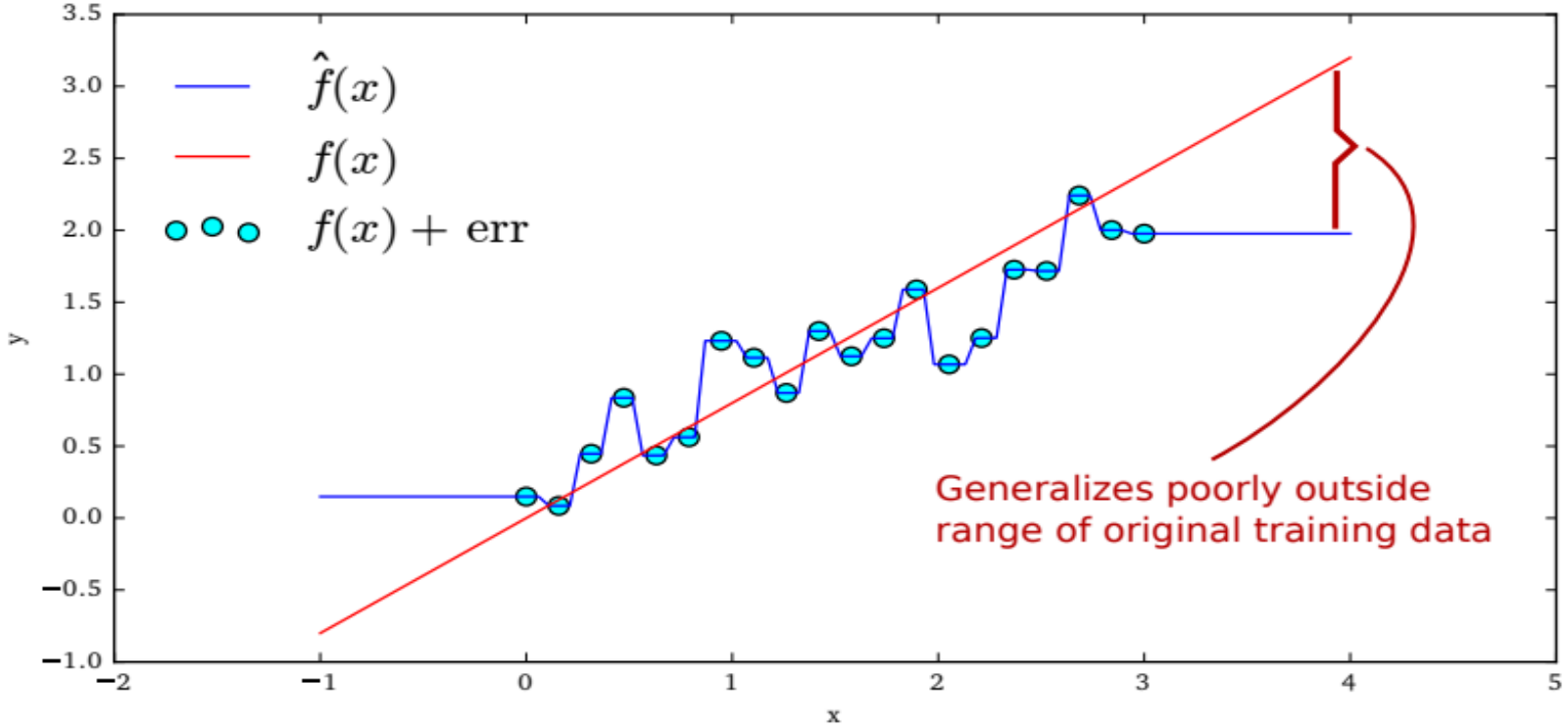
$$d(\mathbf{x}, \mathbf{y}) = \|\mathbf{x} - \mathbf{y}\|_2 = \sqrt{(x_1 - y_1)^2 + (x_2 - y_2)^2}$$

Overfitting



https://www.javatpoint.com/overfitting-in-machine-learning

Nearest neighbours generalisation

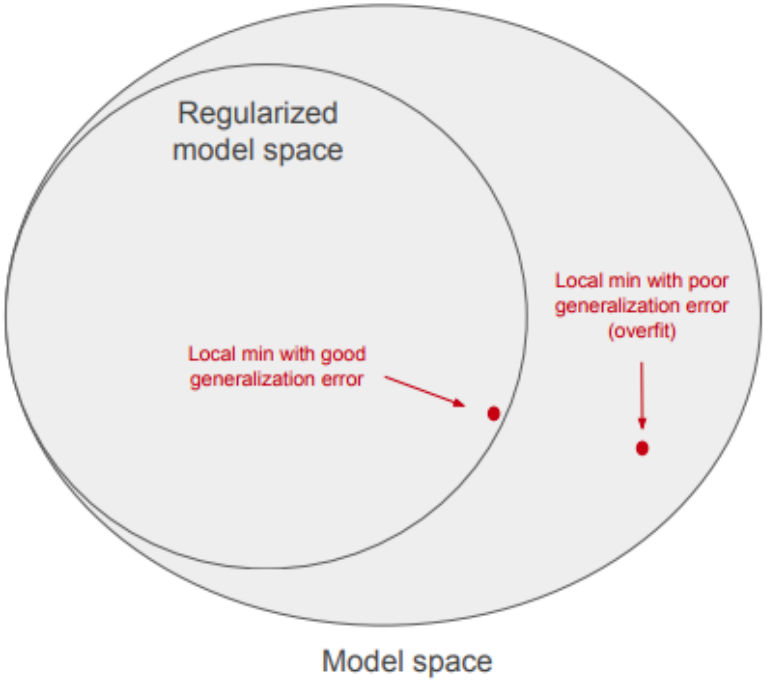


Structural risk minimization

•**Structural risk minimization:** prevent overfitting by balancing model complexity with success at fitting training data.

• Idea: Given two models (hypotheses) with similar training error, prefer ones with lower complexity.

• **Regularization**: add additional information to solve an ill-posed problem or prevent overfitting. Additional information is often a **penalty** included in the loss function.



L2 regularization

Add a penalty to the loss function for large weights.

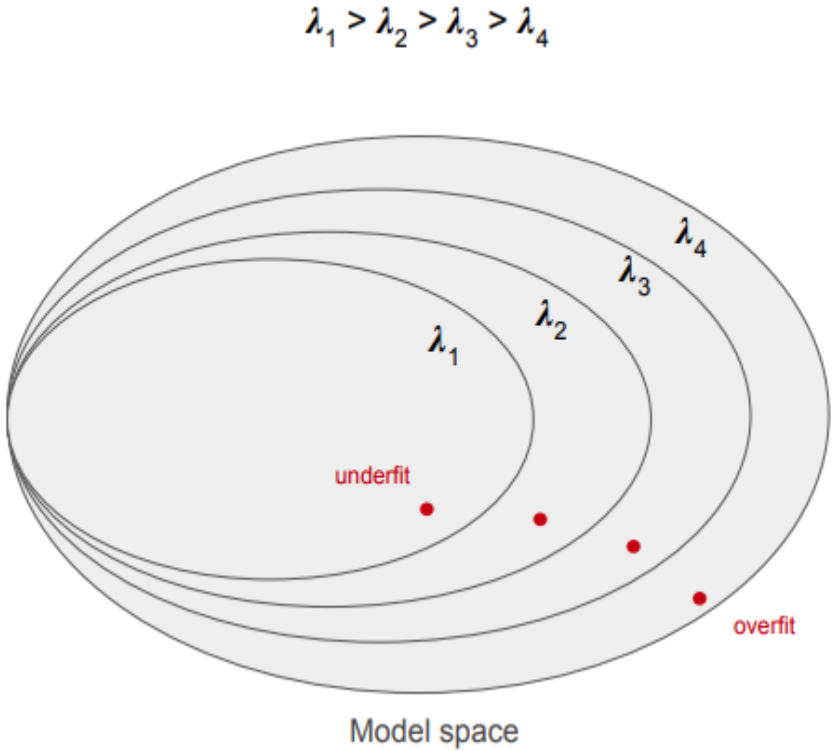
Penalty is on the L_2 norm of the weights

$$\|\mathbf{w}\|_2^2 = \mathbf{w}^T\mathbf{w} = \sum_{i=1}^{D} w_i^2$$

The modified loss is:

$$\mathcal{L} = \mathcal{L}_{\text{data}} + \frac{\lambda}{2}\|\mathbf{w}\|_2^2$$

where λ is the **regularization parameter**, which controls the strength of the regularization



L2 regularization and gradient descent

L_2 regularized loss:

$$\mathcal{L} = \mathcal{L}_{\text{data}} + \frac{\lambda}{2}\|\mathbf{w}\|_2^2$$

Taking the gradient wrt. **w** we get

$$\nabla_{\mathbf{w}}\mathcal{L} = \nabla_{\mathbf{w}}\mathcal{L}_{\text{data}} + \lambda\mathbf{w}$$

which gives the gradient descent update rule:

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha\nabla_{\mathbf{w}}\mathcal{L}_{\text{data}} - \alpha\lambda\mathbf{w}_t$$

This can be understood as slowly *decaying* the weights toward zero with each iteration. In the neural networks literature L_2 regularization is known as **weight decay**.

Why the L2 penalty is reasonable

Imagine we had a training set for which the first two features are always equal $x_1 = x_2$. E.g. this could happen due to a broken sensor, or an image with a watermark.

	x_1	x_2	x_3	x_4	...	x_N	y
$\mathbf{x}_1$	1	1	4	7	...	2	0
$\mathbf{x}_2$	1	1	2	1	...	6	1
$\mathbf{x}_3$	1	1	9	2	...	5	1
:	:	:	:	:	:	:	⋱

If the decision function $f(x) = \mathbf{w}^T\mathbf{x} + b = w_1x_1 + w_2x_2 + \ldots + w_Nx_N + b$, then we can set $w_1 = -w_2$ to any constant we want without changing the outcome or the loss.

Why the L2 penalty is reasonable

Lets say we choose $w_1 = 1000, w_2 = -1000$.

We observe a test point in which $x_2 = 0$. Now we have $f(x) = 1000x_1 + 1000(0) + \ldots$, which changes the value of the decision function by +1000!

With large weights, small changes in input can produce large changes in output!

If we chose $w_1 = w_2 = 0$, the error on the training set would be the same and there would have been no such problem with the test point.

The L_2 penalty encourages finding solutions with **smaller weights**.

Ridge regression

Applying the L_2 penalty to linear regression gives a model called **ridge regression**. The ridge regression loss is:

$$\mathcal{L} = \frac{1}{2}\sum_{i=1}^{N}(y - f(\mathbf{x}))^2 + \frac{\lambda}{2}\|\mathbf{w}\|_2^2$$

The optimal parameters are the solution to

$$\arg\min_{\mathbf{w}} L$$

As with linear regression, this can be solved in closed form by taking derivatives and setting to zero. The solution turns out to be:

$$\hat{\mathbf{w}} = (X^T X + \lambda I)^{-1} X^T \mathbf{y}$$

Choosing the regularization parameter

The regularization parameter λ controls the tradeoff between having small weights and fitting the training data.

- Smaller values for λ place more emphasis on fitting the training data and may be more suitable in low-noise settings or when there are few parameters to fit.
- Larger values for λ place more emphasis on making the values of $\mathbf{w}$ small, and are more suitable when there is a lot of noise or many parameters to fit.

As usual, the best way to choose an appropriate value for λ is using model selection procedures like a hold-out validation set or cross-validation.

Notes on L2 regularization

L_2 regularization is also known as **Tikhonov regularization**.

L_2 regularization in ridge regression corresponds to a Gaussian prior on the weights with zero mean and variance proportional to $1/\lambda$.

Can be used to find least squares solutions to ill-posed problems:

- more free variables than constraints,
- $(X^T X)$ is singular,
- $(X^T X + \lambda I)$ is invertible.

Essential for overparameterized problems like softmax regression.

L1 regularization

L_2 regularization encourages solutions with small weights.

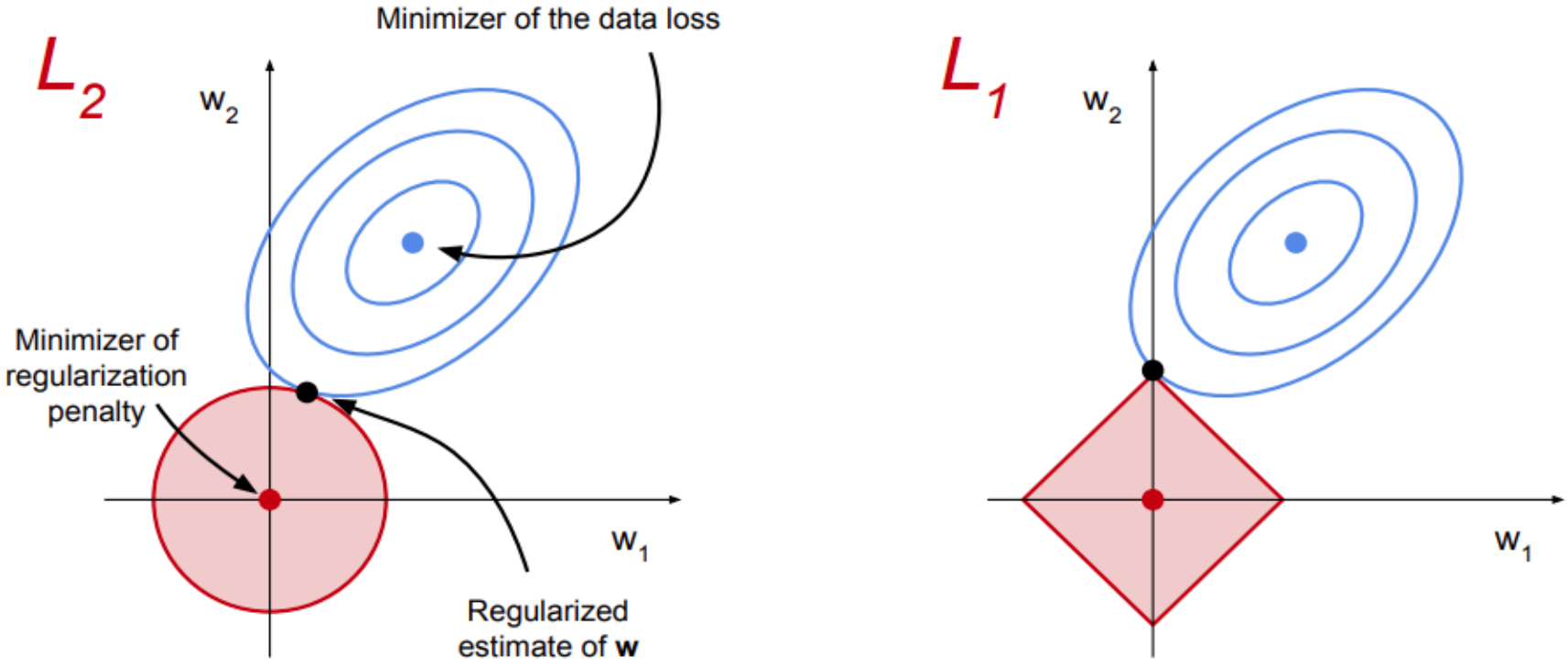
Sometimes you want to find solutions in which most of the weights are exactly zero. These are called **sparse** solutions.

E.g. **feature selection**: you have many features, and you want your decision function to only use a subset. Any feature with weight zero is not used.

L_1 regularization encourages sparse solutions by using penalizing the L_1-norm of the weights.

$$\|\mathbf{w}\|_1 = \sum_{i=1}^{D} |w_i|$$

How does L1 regularization encourage sparsity?



(Sub)-gradient descent for L1 regularization

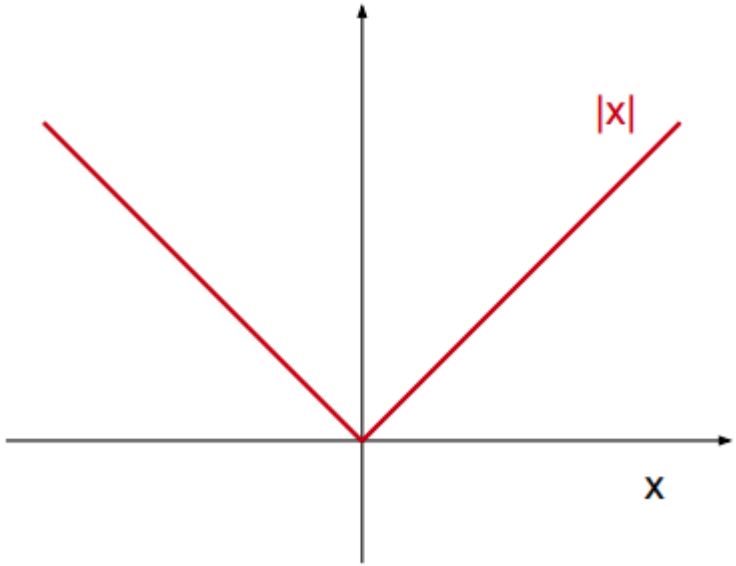
L_1 regularized loss:

$$\mathcal{L} = \mathcal{L}_{\text{data}} + \lambda \|\mathbf{w}\|_1$$

$$= \mathcal{L}_{\text{data}} + \lambda \sum_{i=1}^{D} |w_i|$$

The absolute value has a discontinuity at zero so gradient is not defined everywhere.

For gradient descent we can use a **subgradient**.



(Sub)-gradient descent for L1 regularization

A subgradient for $|w|$ is:

$$\nabla_w |w| = \begin{cases} 1 & w > 0 \\ -1 & w < 0 \\ 0 & w = 0 \end{cases}$$

which can be written more succinctly using the sign function $\nabla_w |w| = \text{sign}(w)$.

This gives us the subgradient descent update rule for L_1 regularization:

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha \nabla_{\mathbf{w}} \mathcal{L} - \lambda \sum_{i=0}^{D} \text{sign}(w_i)$$

The LASSO and Elastic Net

Combining ordinary least squares regression with the L_1 penalty gives rise to the so called **LASSO** (least absolute shrinkage and selection operator).

Can solve using subgradient descent as shown. Generally preferable to use a faster algorithm like **least angle regression** (LARS).

It is also possible to use **both** L_1 and L_2 regularizers together. This model is called the **elastic net**.

In scikit-learn

- sklearn.linear model.Ridge
- sklearn.linear model.Lasso
- sklearn.linear model.LassoLars
- sklearn.linear model.ElasticNet

Logistic regression in scikit-learn can also take an L_1 or L_2 regularization penalty: LogisticRegression(penalty='l2', C=1.0), where $C > 0$ is the **inverse** of λ (smaller values specify stronger regularization).

Scikit-learn also has classes that do automatic (and optimized) cross validation to figure out the best value for the regularization parameter(s). E.g.:

- sklearn.linear model.RidgeCV
- sklearn.linear model.LassoCV

Resources

Stanford machine learning lectures (Andrew Ng):

- Lecture 3: linear and logistic regression
  http://www.youtube.com/watch?v=HZ4cvaztQEs
- Lecture 4: Generalized linear models
  http://www.youtube.com/watch?v=nLKOQfKLUks

Caltech machine learning lectures (Yaser Abu-Mostafa):

- Lecture 12: Regularization
  http://www.youtube.com/watch?v=I-VfYXzC5ro

Resources

Oxford deep learning lectures (Nando de Freitas):

- Lecture 4: Regularization 1
  http://www.youtube.com/watch?v=VR0W_PNwLGw
- Lecture 5: Regularization 2
  http://www.youtube.com/watch?v=VR0W_PNwLGw