# **Learning and Linear Regression**

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# **Linear Regression 1: Best Line**

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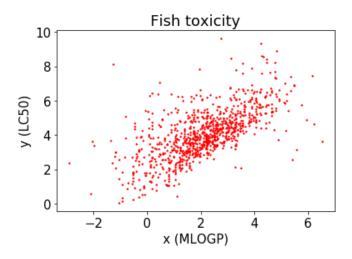
Let's understand *linear regression* as a type of machine learning. Let's consider

as a sample dataset.

		CIC0	SM1_Dz(Z)	GATS1i	NdsCH	NdssC	MLOGP	LC50
Ī	0	3.260	0.829	1.676	0	1	1.453	3.770
	1	2.189	0.580	0.863	0	0	1.348	3.115
	2	2.125	0.638	0.831	0	0	1.348	3.531
	3	3.027	0.331	1.472	1	0	1.807	3.510
	4	2.094	0.827	0.860	0	0	1.886	5.390

We want to understand how an  $\mathbb{R}$ -valued *response* (y) depends on an  $\mathbb{R}$ -valued *feature* (x) (perhaps one of several possible features) We have N test datapoints which we want to *learn* from.

feature (x): MLOGP response (y): LC50 N=908

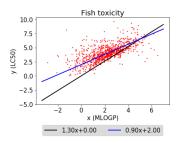


The scatterplot sort of clusters around a line

We want to model the data as

$$y = \underbrace{mx + b}_{\ell_{m,b}(x)}$$

where  $\ell_{m,b}$  is a line parametrized by slope m and y-intercept b. Instead of fixing the parameters m and b and studying  $\ell_{m,b}$ , we are here given N datapoints  $\{(x_n,y_n)\}_{n=1}^N$  and one tries to *learn* m and b.

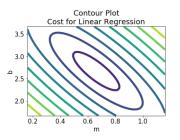


We want to find the parameters *m* and *b* which *best* explain the data.

We quantify best by writing down the the error as a cost function

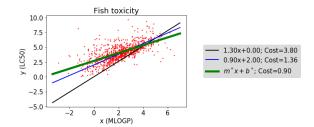
$$\Lambda(m,b) \stackrel{\text{def}}{=} \frac{1}{N} \sum_{n=1}^{N} \underbrace{\left(\underbrace{y_n - \ell_{m,b}(x_n)}_{\theta_n(m,b)}\right)^2}_{\theta_n(m,b)}$$

(the mean square error) and then minimizing over  $(m, b) \in \mathbb{R}^2$ .



$$\Lambda(m^*,b^*)=\min_{(m,b)\in\mathbb{R}^2}\Lambda(m,b).$$

$$m^* = 0.66$$
  
 $b^* = 2.67$   
minimal cost=1.22



note: The cost function  $\Lambda$  can be understood as the *variance* of the error

$$y_n = mx_n + b + ERROR_n$$

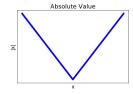
if the ERROR $_n$ 's are statistically independent and identically distributed random variables.

## **Metrics**

Once we have identified the "best" parameters  $(m^*, b^*)$  (which minimize C), we can then compute a *metric* 

$$\mu_{\text{metric}} \stackrel{\text{def}}{=} \frac{1}{N} \sum_{n=1}^{N} \left| \underbrace{y_n - \ell_{m^*,b^*}(x_n)}_{\varepsilon_n(m^*,b^*)} \right|$$

$$\mu_{metric} = 0.82$$



which tells us how good our machine learning procedure turned out to be. In this case, the metric  $\boldsymbol{\mu}$ 

- Is not differentiable ( $x \mapsto |x|$  fails to be differentiable at 0)
- Lacks the statistical appeal of the cost function *C*.

## **Metrics vs Costs**

### Generally,

- The *metric* often reflects statistical assessment. The *cost* function tries to capture the idea of the metric, but is regular enough to (efficiently) apply (robust) optimization algorithms.
- There are range of existing costs and metrics for existing problems. Costs and metrics for new problems are something of an art. A cost is a "good enough" approximation of metric, where "good enough" respects the fact that meaningful applications of machine learning often have noise and complex structure (as opposed to mathematical models).

## **Summary**

## Let's write down some salient points:

- We have a set  $\{(\text{feature}_n, \text{response}_n)\}_{n=1}^N$  of *ground truth* datapoints which we will use to *supervise* our efforts.
- We have a  $model \, \ell_{m,b}$  of the feature-response relationship; this model depends on a finite collection of model parameters. which we want to identify
- We have a *cost* function  $\Lambda$  which quantifies the error (between the model and the ground truth data) as a function of the model parameters. This cost can further be broken down as a sum of cost functions for each data point (the  $\theta_n$ 's). We want to minimize this cost function over choices of the model parameters.
- We have a metric which quantifies how well we are able to express the ground truth in terms of the optimal model.



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# **Linear Regression 2: Cost Function**

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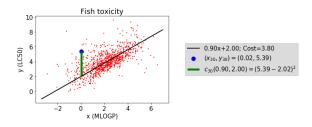




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## **Mathematics of Cost Function**

Let's look a bit more closely at the  $\theta_n$ 's. Each  $\theta_n(m,b)$  is the square of the vertical distance  $\varepsilon_n(m,b)$  from the line  $\ell_{m,b}$  to the point  $(x_n,y_n)$ .



$$(x_{30}, y_{30}) = (0.02, 5.39)$$
  
 $c_{30}(m, b) = (5.39 - 0.02m - b)^2$ 

Mathematically,

$$\begin{array}{ll}
\mathbf{p} = \begin{pmatrix} m \\ b \end{pmatrix} \\
= \text{parameters of model} \\
\widehat{\varepsilon}_n(m, b) &= y_n - mx_n - b = y_n - \overbrace{(x_n \quad 1)}^{\mathbf{X}_n^T} \begin{pmatrix} m \\ b \end{pmatrix} \\
\theta_n(\mathbf{p}) = (\varepsilon_n(\mathbf{p}))^2
\end{array}$$

The augmented feature variable

$$\mathbf{X}_n \stackrel{\text{def}}{=} \begin{pmatrix} x_n \\ 1 \end{pmatrix}$$

allows us to efficiently consider shifts in the data.

We claim that  $\theta_n$  is *convex* in **p**; i.e., for any **p**<sub>1</sub> and **p**<sub>2</sub> in  $\mathbb{R}^2$  and  $\theta \in [0, 1]$ ,

$$\underbrace{\begin{split} \boldsymbol{\varepsilon}_{n}}_{\text{affine}} (\theta \mathbf{p}_{1} + (1 - \theta) \mathbf{p}_{2}) &= y_{n} - \mathbf{X}_{n}^{T} \{\theta \mathbf{p}_{1} + (1 - \theta) \mathbf{p}_{2} \} \\ &= y_{n} - \theta \mathbf{X}_{n}^{T} \mathbf{p}_{1} - (1 - \theta) \mathbf{X}_{n}^{T} \mathbf{p}_{2} \\ &= \theta \{ y_{n} - \mathbf{X}_{n}^{T} \mathbf{p}_{1} \} + (1 - \theta) \{ y_{n} - \mathbf{X}_{n}^{T} \mathbf{p}_{2} \} \\ &= \theta \varepsilon_{n}(\mathbf{p}_{1}) + (1 - \theta) \varepsilon_{n}(\mathbf{p}_{2}) \\ \theta_{n} (\theta \mathbf{p}_{1} + (1 - \theta) \mathbf{p}_{2}) &= \underbrace{(\theta \varepsilon_{n}(\mathbf{p}_{1}) + (1 - \theta) \varepsilon_{n}(\mathbf{p}_{2}))^{2}}_{f(\theta)} \end{split}$$

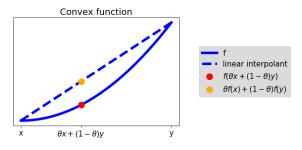
Then

$$f(\theta) = (\varepsilon_n(\mathbf{p}_2) + \theta \{\varepsilon_n(\mathbf{p}_1) - \varepsilon_n(\mathbf{p}_2)\})^2$$

$$f'(\theta) = 2(\varepsilon_n(\mathbf{p}_2) + \theta \{\varepsilon_n(\mathbf{p}_1) - \varepsilon_n(\mathbf{p}_2)\}) \{\varepsilon_n(\mathbf{p}_1) - \varepsilon_n(\mathbf{p}_2)\}$$

$$f''(\theta) = 2\{\varepsilon_n(\mathbf{p}_1) - \varepsilon_n(\mathbf{p}_2)\}^2 \ge 0$$

Since  $f'' \ge 0$ , f' is nondecreasing, so f should be convex.



$$f(\theta) - f(0) = \int_{s=0}^{\theta} f'(s) ds \le f'(\theta) \theta$$
  
$$f(1) - f(\theta) = \int_{s=\theta}^{1} f'(s) ds \ge f'(\theta) (1 - \theta);$$

thus

$$\theta \{f(1) - f(\theta)\} \ge f'(\theta)\theta(1 - \theta) \ge (1 - \theta)\{f(\theta) - f(0)\}$$

which can be rearranged as

$$\underbrace{\theta f(1) + (1-\theta)f(0)}_{\theta\theta_n(\mathbf{p}_1) + (1-\theta)\theta_n(\mathbf{p}_2)} \ge \theta f(\theta) + (1-\theta)f(\theta) = \underbrace{f(\theta)}_{\theta_n(\theta\mathbf{p}_1 + (1-\theta)\mathbf{p}_2)}$$

Since each  $\theta_n$  is convex,

$$\frac{1}{N} \sum_{n=1}^{N} \underbrace{\frac{\theta_n(\theta \mathbf{p}_1 + (1-\theta)\mathbf{p}_2)}{f_n(\theta)}} \\
\leq \frac{1}{N} \sum_{n=1}^{N} \left\{ \underbrace{\theta \underbrace{\theta_n(\mathbf{p}_2)}_{f_n(0)} + (1-\theta) \underbrace{\theta_n(\mathbf{p}_1)}_{f_n(1)}}_{\theta_n(\mathbf{p}_1)} \right\} \\
= (1-\theta) \underbrace{\frac{1}{N} \sum_{n=1}^{N} \theta_n(\mathbf{p}_2)}_{\Lambda(\mathbf{p}_2)} + (1-\theta) \underbrace{\frac{1}{N} \sum_{n=1}^{N} \theta_n(\mathbf{p}_1)}_{\Lambda(\mathbf{p}_1)}$$

so  $\Lambda$  is also convex.

Convex functions are nice; if

$$\underbrace{\min_{\boldsymbol{p} \in \mathbb{R}^2} \Lambda(\boldsymbol{p})}_{\underline{\mathcal{C}}} = \Lambda(\boldsymbol{p}_1^*) = \Lambda(\boldsymbol{p}_2^*) \qquad \text{(two minimizers)}$$

then for any  $\theta \in [0, 1]$ ,

$$\underbrace{\frac{\min\limits_{\boldsymbol{p}\in\mathbb{R}^2}\Lambda(\boldsymbol{p})}{\underline{C}}}_{\underline{C}} \leq \Lambda\left(\theta\boldsymbol{p}_1^* + (1-\theta)\boldsymbol{p}_2^*\right)$$

$$\leq \theta\underbrace{\Lambda(\boldsymbol{p}_2^*)}_{=\underline{C}} + (1-\theta)\underbrace{\Lambda(\boldsymbol{p}_1^*)}_{=\underline{C}} = \underline{C}$$

so

$$\Lambda \left(\theta \mathbf{p}_1^* + (1-\theta)\mathbf{p}_2^*\right) = \underline{C};$$

the set of minimizers is convex (and thus connected).

If  $\Lambda$  is *strictly* convex, inequalities are strict, leading to a contradiction if the set of minimizer is not unique.

Let's next look at level sets of  $\varepsilon_n$  (and thus  $\theta_n$ ). For any  $\mathbf{p} \in \mathbb{R}^2$  and any  $\alpha \in \mathbb{R}$ ,

$$\varepsilon_{n} \left( \mathbf{p} + \alpha \underbrace{\begin{pmatrix} \mathbf{1} \\ -X_{n} \end{pmatrix}}_{\mathbf{X}_{n}^{\perp}} \right) = y_{n} - \mathbf{X}_{n}^{T} \left\{ \mathbf{p} + \alpha \mathbf{X}_{n}^{\perp} \right\}$$

$$= \underbrace{y_{n} - \mathbf{X}_{n}^{T} \mathbf{p}}_{\varepsilon_{n}(\mathbf{p})} - \underbrace{\alpha \mathbf{X}_{n}^{T} \mathbf{X}_{n}^{\perp}}_{(X_{n} - 1) \begin{pmatrix} \mathbf{1} \\ -X_{n} \end{pmatrix}}_{=0}$$

SO

$$\theta_n \left( \mathbf{p} + \alpha \mathbf{X}_n^{\perp} \right) = \left( \varepsilon_n \left( \mathbf{p} + \alpha \mathbf{X}_n^{\perp} \right) \right)^2 = \left( \varepsilon_n(\mathbf{p}) \right)^2$$

i.e.,  $\theta_n$  is constant along displacements in the direction of  $\mathbf{X}_n^{\perp}$  (and thus  $\theta_n$  is not strictly convex).

We can graphically understand

$$\left\{\mathbf{p}\in\mathbb{R}^2: heta_n(\mathbf{p})=1.44
ight\};$$

cost is square of vertical distance from  $(x_n, y_n)$  to line with parameters  $\mathbf{p} = (m, b)$ .  $\theta_n(\mathbf{p}) = 1.44 (= 1.2^2)$  corresponds to a line (of some slope m) passing through  $(x_n, y_n \pm 1.2)$ . A line of slope m passing through  $(x_n, y_n \pm 1.2)$  is given by (point-slope formula)

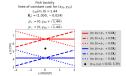
$$\frac{y-(y_n\pm 1.2)}{x-x_n}=m;$$

namely

$$y = mx + \underbrace{\{y_n \pm 1.2 - mx_n\}}_{h}$$

SO

$$\mathbf{p} = \begin{pmatrix} m \\ b \end{pmatrix} = \begin{pmatrix} m \\ y_n \pm 1.2 - mx_n \end{pmatrix} = \begin{pmatrix} 0 \\ y_n \pm 1.2 \end{pmatrix} + m \underbrace{\begin{pmatrix} 1 \\ -x_n \end{pmatrix}}_{\mathbf{y} \perp}$$



We can explicitly compute Hessian of costs;

$$\theta_n(\mathbf{p}) = (y_n - \mathbf{X}_n^T \mathbf{p})^2$$

 $(\theta_n \text{ is quadratic in } \mathbf{p}); \theta_n \text{ has Hessian}$ 

$$\underbrace{\mathbf{X}_{n}\mathbf{X}_{n}^{T}}_{Q_{n}} = \begin{pmatrix} x_{n} \\ 1 \end{pmatrix} \begin{pmatrix} x_{n} & 1 \end{pmatrix} = \begin{pmatrix} x_{n}^{2} & x_{n} \\ x_{n} & 1 \end{pmatrix}$$

- lacksquare  $Q_n$  has rank one ( $\mathbf{X}_n^{\perp}$  is in kernel), although it is  $2 \times 2$
- $\blacksquare$   $Q_n$  is symmetric
- $\blacksquare Q_n \geq 0$ ;  $\mathbf{p}^T Q_n \mathbf{p} = (\mathbf{X}_n^T \mathbf{p})^2 \geq 0$  for any  $\mathbf{p} \in \mathbb{R}^2$ .

#### Thus Λ has Hessian

$$Q \stackrel{\text{def}}{=} \frac{1}{N} \sum_{n=1}^{N} Q_n = \frac{1}{N} \sum_{n=1}^{N} \begin{pmatrix} x_n^2 & x_n \\ x_n & 1 \end{pmatrix}$$

- $\blacksquare$  Q is full rank (unless all  $x_n$ 's agree)
- Q is symmetric
- **■**  $Q_n \ge 0$ ;  $\mathbf{p}^T Q \mathbf{p} = \frac{1}{N} \sum_{n=1}^N \mathbf{p}^T Q_n \mathbf{p} \ge 0$  for any  $\mathbf{p} \in \mathbb{R}^2$ .

## **Summary**

- The cost function  $\Lambda$  can be written as an average of cost functions  $\theta_n$ , where each  $\theta_n$  is a cost between the model and a single record.
- Each  $\theta_n$  is convex;  $\Lambda$  is thus convex (and typically strictly convex).



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# **Linear Regression 3: Minimal Cost**

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Linear regression has an explicit solution, given by the Euler equations of optimality. Let's perturb the optimal  $\mathbf{p}^*$  by amount  $\delta \in \mathbb{R}$  in direction  $\tilde{\mathbf{p}}$ .

$$\varepsilon_n(\mathbf{p}^* + \delta \tilde{\mathbf{p}}) = y_n - \mathbf{X}_n^T \{ \mathbf{p}^* + \delta \tilde{\mathbf{p}} \} = \underbrace{y_n - \mathbf{X}_n^T \mathbf{p}^*}_{\varepsilon_n(\mathbf{p}^*)} - \delta \mathbf{X}_n^T \tilde{\mathbf{p}}$$

SO

$$\Lambda(\mathbf{p}^* + \delta \tilde{\mathbf{p}}) = \frac{1}{N} \sum_{n=1}^{N} \left( \varepsilon_n(\mathbf{p}^*) - \delta \mathbf{X}_n^T \tilde{\mathbf{p}} \right)^2.$$

Taking derivatives with respect to  $\delta$ ,

$$\underbrace{\frac{D\Lambda(\mathbf{p}^*)\tilde{\mathbf{p}}}{\text{principle}}}_{\text{derivative at }\mathbf{p}^* \text{ in direction }\tilde{\mathbf{p}} \in \mathbb{R}^2} = -2\frac{1}{N}\sum_{n=1}^N \varepsilon_n(\mathbf{p}^*)\mathbf{X}_n^T\tilde{\mathbf{p}}$$

$$\underbrace{D\Lambda(\mathbf{p}^*)}_{\text{leaves a from }\mathbb{P}^2} = -2\frac{1}{N}\sum_{n=1}^N \varepsilon_n(\mathbf{p}^*)\mathbf{X}_n^T$$

The Euler condition of optimality is that if

$$\Lambda(\mathbf{p}^*) = \min_{\mathbf{p} \in \mathbb{R}^2} \Lambda(\mathbf{p})$$

then

$$0 = D\Lambda(\mathbf{p}^*) = -2\frac{1}{N} \sum_{n=1}^{N} \underbrace{\left\{y_n - \mathbf{X}_n^T \mathbf{p}^*\right\}}_{\varepsilon_n(\mathbf{p}^*)} \mathbf{X}_n^T$$

which can be rearranged ( $\mathbf{X}_n^T \mathbf{p}^* = \mathbf{p}^{*,T} \mathbf{X}_n$  is a scalar) as

$$\underbrace{\frac{1}{N}\sum_{n=1}^{N}y_{n}\mathbf{X}_{n}}_{\mathbf{v}} = \underbrace{\frac{1}{N}\sum_{n=1}^{N}\mathbf{X}_{n}\mathbf{X}_{n}^{T}\mathbf{p}^{*}}_{Q}$$

SO

$${\bf p}^* = Q^{-1}{\bf v}.$$

This agrees with standard formulæ.

$$\mathbf{v} = \frac{1}{N} \sum_{n=1}^{N} \begin{pmatrix} y_n x_n \\ y_n \end{pmatrix} = \begin{pmatrix} \overline{x} \overline{y} \\ \overline{y} \end{pmatrix}$$

$$Q = \frac{1}{N} \sum_{n=1}^{N} \begin{pmatrix} x_n \\ 1 \end{pmatrix} (x_n \quad 1) = \frac{1}{N} \sum_{n=1}^{N} \begin{pmatrix} x_n^2 & x_n \\ x_n & 1 \end{pmatrix}$$

$$= \begin{pmatrix} \overline{x^2} & \overline{x} \\ \overline{x} & 1 \end{pmatrix}$$

where - empirically averages.

Then

$$\begin{split} \begin{pmatrix} m^* \\ b^* \end{pmatrix} &= \underbrace{\frac{\mathbf{p}^*}{\mathbf{p}^{-1}\mathbf{v}}} = \frac{1}{\overline{x^2} - \overline{x}^2} \begin{pmatrix} 1 & -\overline{x} \\ -\overline{x} & \overline{x^2} \end{pmatrix} \begin{pmatrix} \overline{y}\overline{x} \\ \overline{y} \end{pmatrix} \\ &= \begin{pmatrix} \frac{\overline{x}\overline{y} - \overline{x} \cdot \overline{y}}{\overline{x^2} - \overline{x}^2} \\ -\overline{x} \cdot \overline{x}\overline{y} + \overline{x^2}\overline{y} \\ \overline{x^2} - \overline{x}^2 \end{pmatrix} = \begin{pmatrix} \frac{\overline{x}\overline{y} - \overline{x} \cdot \overline{y}}{\overline{x^2} - \overline{x}^2} \\ -\overline{x} \{\overline{x}\overline{y} - \overline{x} \cdot \overline{y} + \{\overline{x^2} - \overline{x}^2\}\overline{y} \end{pmatrix} \\ &= \begin{pmatrix} \frac{\overline{x}\overline{y} - \overline{x} \cdot \overline{y}}{\overline{x^2} - \overline{x}^2} \\ -\overline{x} \frac{\overline{x}\overline{y} - \overline{x} \cdot \overline{y}}{\overline{x^2} - \overline{x}^2} + \overline{y} \end{pmatrix} \end{split}$$

The regression line is thus the well-known formula

$$\ell_{m^*,b^*}(x) = m^*x + b^* = \frac{\overline{xy} - \overline{x} \cdot \overline{y}}{\overline{x^2} - \overline{x}^2} x - \overline{x} \frac{\overline{xy} - \overline{x} \cdot \overline{y}}{\overline{x^2} - \overline{x}^2} + \overline{y}$$

$$= \overline{y} + \underbrace{\frac{\overline{xy} - \overline{x} \cdot \overline{y}}{\overline{x^2} - \overline{x}^2}}_{= \frac{\text{Covariance}(x,y)}{\text{Variance}(x)}} (x - \overline{x})$$

## **Z-scores**

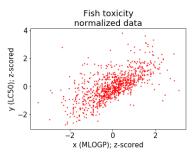
By first subtracting the mean and then dividing by standard deviation (i.e., taking *z-scores*), we can normalize datasets to be mean zero and unit standard deviation, leading to better numerical stability.

$$\sigma_{X,X} \stackrel{\text{def}}{=} \overline{(x-\overline{x})^2}; \quad \sigma_{Y,Y} \stackrel{\text{def}}{=} \overline{(y-\overline{y})^2}; \quad \sigma_{X,Y} \stackrel{\text{def}}{=} \overline{(x-\overline{x})(y-\overline{y})}.$$

then

$$X_n^z \stackrel{\text{def}}{=} \frac{X_n - \overline{X}}{\sqrt{\sigma_{X,X}}} \qquad y_n^z \stackrel{\text{def}}{=} \frac{y_n - \overline{y}}{\sqrt{\sigma_{Y,Y}}}$$

Then  $\{(x_n^z, y_n^z)\}_{n=1}^N$  is centered at the origin and has unit standard deviation in the x and y directions.



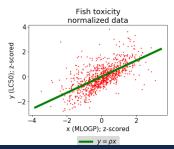
Our original formula for regression was

$$\ell_{m^*,b^*}(x) = \overline{y} + \frac{\sigma_{X,Y}}{\sigma_{X,X}}(x - \overline{x})$$

which we can rewrite as

$$\frac{\ell_{m^*,b^*}(x) - \overline{y}}{\sqrt{\sigma_{Y,Y}}} = \underbrace{\frac{\sigma_{X,Y}}{\sqrt{\sigma_{Y,Y}}\sqrt{\sigma_{X,X}}}}_{\text{z-score of response}} \underbrace{\left(\frac{X - \overline{X}}{\sqrt{\sigma_{X,X}}}\right)}_{\text{z-score of feature}} \underbrace{\left(\frac{X - \overline{X}}{\sqrt{\sigma_{X,X}}}\right)}_{\text{correlation coefficient between X and Y}} (+0)$$

regressed offset b for z-scored data: 1.01e-16 regressed slope m for z-scored data: 0.652 correlation coefficient for z-scored data: 0.652





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# **Linear Regression 4. Gradient Descent**

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$$D\Lambda(\mathbf{p}) = -2\frac{1}{N}\sum_{n=1}^{N}\varepsilon_{n}(\mathbf{p})\mathbf{X}_{n}^{T}.$$

can convert derivative to gradient through duality on  $\mathbb{R}^2$  with standard inner product  $\langle x, y \rangle = x^T y$ ;

$$\langle \nabla \Lambda(\boldsymbol{p}), \boldsymbol{\tilde{p}} \rangle = \underbrace{D \Lambda(\boldsymbol{p})}_{(\nabla \Lambda(\boldsymbol{p}))^T} \boldsymbol{\tilde{p}}$$

so

$$\nabla \Lambda(\mathbf{p}) = -2\frac{1}{N} \sum_{n=1}^{N} \varepsilon_n(\mathbf{p}) \mathbf{X}_n$$

For  $\delta > 0$  small,

$$\begin{split} \Lambda\left(\mathbf{p} - \delta\nabla\Lambda(\mathbf{p})\right) &\approx \Lambda(\mathbf{p}) - \delta D\Lambda(\mathbf{p})\nabla\Lambda(\mathbf{p}) = \Lambda(\mathbf{p}) - \delta\left\langle\nabla\Lambda(\mathbf{p}), \nabla\Lambda(\mathbf{p})\right\rangle \\ &= \Lambda(\mathbf{p}) - \delta\|\nabla\Lambda(\mathbf{p})\|_{\mathbb{R}^2}^2 \leq \Lambda(\mathbf{p}) \end{split}$$

Gradient descent is

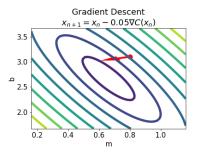
$$\mathbf{p}_{n+1} = \mathbf{p}_n - \delta \nabla \Lambda(\mathbf{p}_n)$$

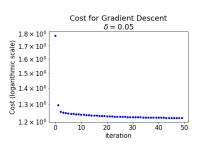
At minimum **p**\*,

$$D\Lambda(\mathbf{p}^*) = 0 \Leftrightarrow \nabla\Lambda(\mathbf{p}^*) = 0 \Leftrightarrow \text{Euler conditions}$$

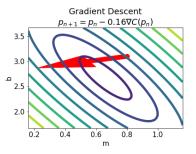
(if not at extremal,  $\nabla \Lambda(\mathbf{p}) \neq 0$ ).

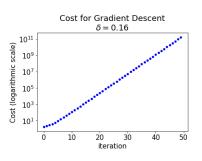
## Converges for $\delta \ll 1$ (but perhaps slowly)





### Diverges for $\delta \gg 1$ (overshoots)





More advanced algorithms modify gradient descent to improve performance. Python scipy.optimize.minimize has

- Nelder-Mead
- Conjugate-gradient
- Broyden, Fletcher, Goldfarb, and Shanno (BFGS)
- Newton-Conjugate-Gradient
- dog-leg trust-region
- Newton conjugate gradient trust-region
- Newton Generalized Lanczos trust-region



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