Statistics and Data Science 365 / 565

Data Mining and Machine Learning

February 6

Yale

Outline

- Recap: supervised learning goal
- How do we assess if we've learned well?
- Training vs testing
- Linear Regression
- Quadratic Regression
- Kernel Regression
- KNN regression
- Notebook

Recap: Supervised learning goals

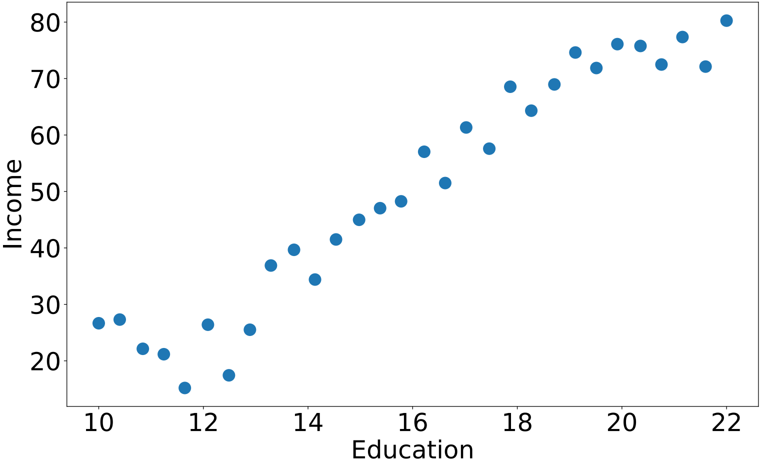
Create a function $\widehat{f} : \mathcal{X} \mapsto \mathcal{Y}$ by “learning” from data $z_i = (x_i, y_i)$.

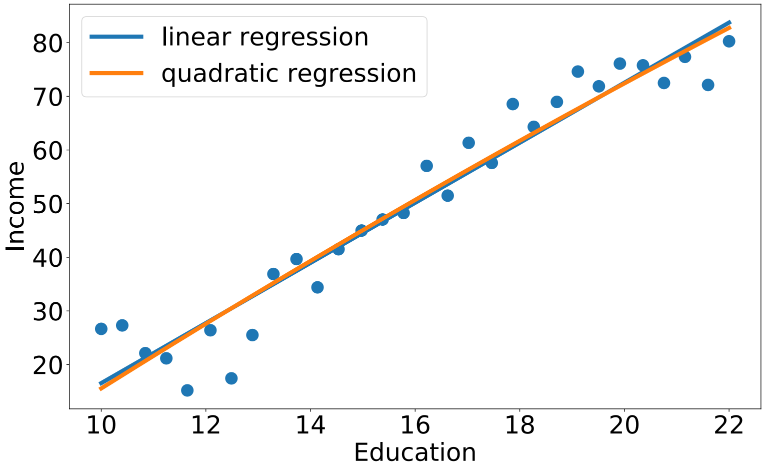
Probably want $\widehat{f}(x_i) \approx y_i$ (Notation: $\approx$ means approximately)

Regression: $\mathcal{Y}$ is continuous/ordered (prices)

Classification: $\mathcal{Y}$ is discrete/unordered (labels: hot dog v not hot dog)

Lots of approaches


80
70
60
50
40
30
20
Income
10
12
14
16
18
20
22
Education


linear regression
quadratic regression
Income
Education
80
70
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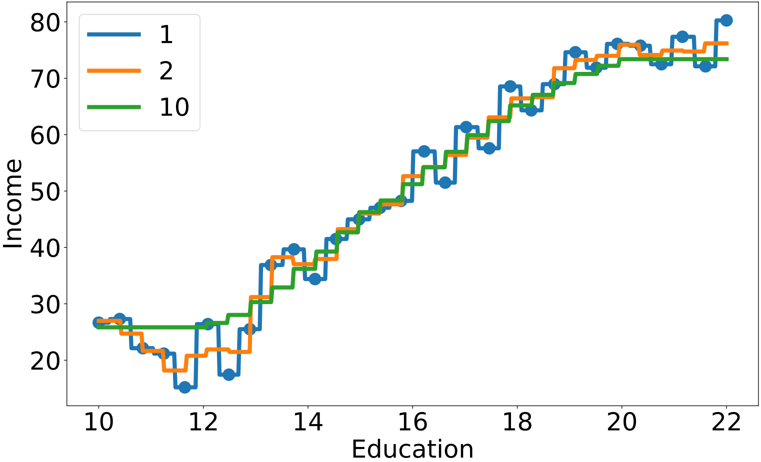
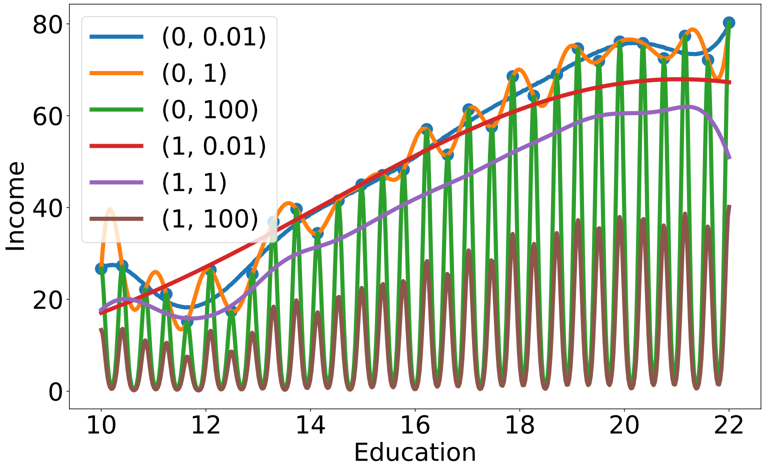
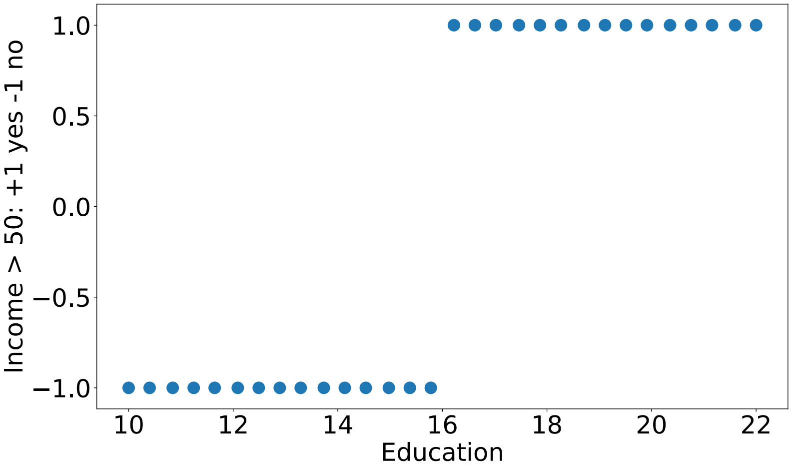
Nearest neighbor

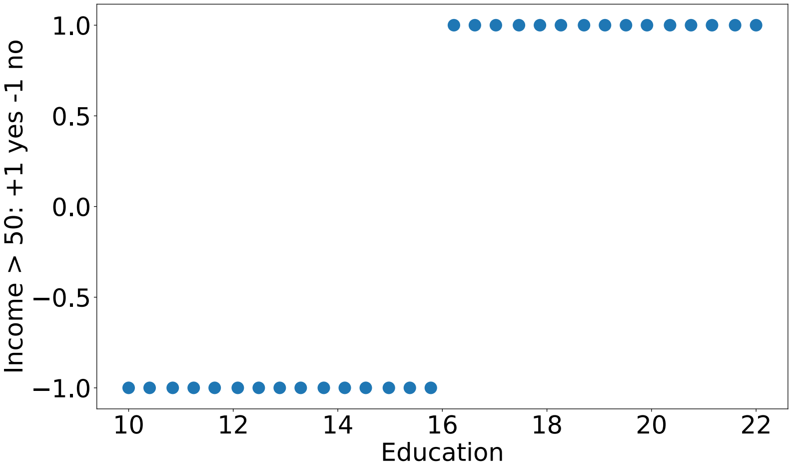
Estimate answer of unseen point by averaging neighbors





(0, 0.01)
(0, 1)
(0, 100)
(1, 0.01)
(1, 1)
(1, 100)
Income
0
20
40
60
80
Education
10
12
14
16
18
20
22


1.0
0.5
0.0
−0.5
−1.0
Income > 50: +1 yes -1 no
10
12
14
16
18
20
22
Education



Income > 50: +1 yes -1 no
1.0
0.5
0.0
−0.5
−1.0
10
12
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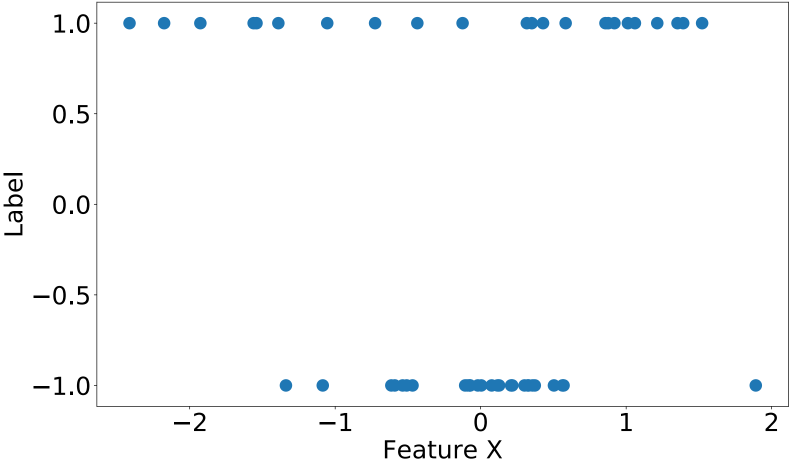
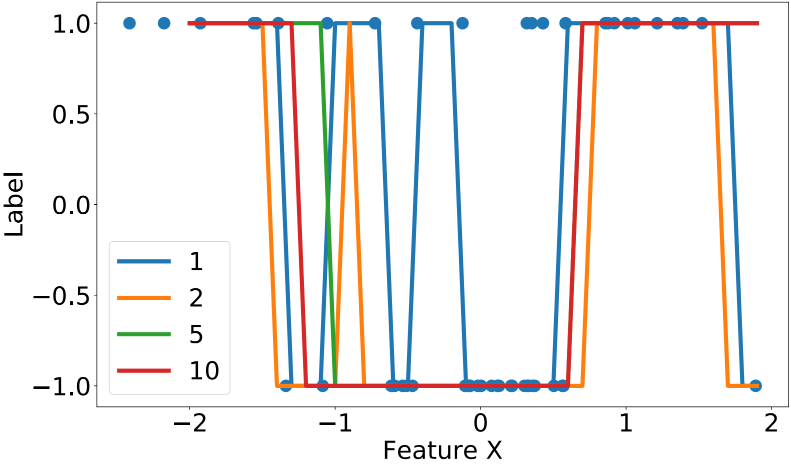
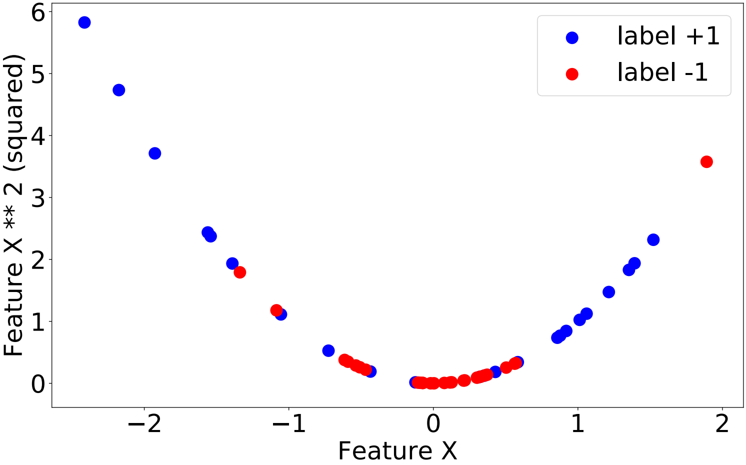
20
22
Education


Label
Feature X
1.0
0.5
0.0
−0.5
−1.0
−2
−1
0
1
2


1.0
0.5
0.0
−0.5
−1.0
Label
−2
−1
0
1
2
Feature X
1
2
5
10



label +1
label -1
Feature X ** 2 (squared)
Feature X
0
1
2
3
4
5
6
−2
−1
0
1
2

Loss

How do we check how well $f(x) \approx y$ for a specific example?

One way (of many reasonable approaches): Write loss as $\ell(y', y)$: y' prediction, y truth for example features x. This is more "Frequentist" will see "Bayesian" way later

Classification:

Hamming $0/1$ loss: $\mathbb{1}(y' \neq y)$

Notation:

$$\mathbb{1}(A) = \begin{cases} 1 & \text{if } A \text{ is true} \\ 0 & \text{if } A \text{ is false} \end{cases}$$

Loss

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One way (of many reasonable approaches): Write loss as $\ell(y', y)$: y' prediction, y truth for example features x. This is more “Frequentist” will see “Bayesian” way later

Regression:

Squared loss: $(y - y')^2$

Absolute loss: $|y - y'|$

Choice of loss has implications. Explore in next pset.

How to combine over all data? Empirical risk of function f

$$\widehat{R}(f) = \frac{1}{n}\sum_{i=1}^{n} \ell(f(x_i), y_i)$$

Doing so carries a lot of implications (everything weighted the same, bias towards majority group of data, ...), but it's a good place to start.

$\ell(y', y)$	$\widehat{R}$ name
$(y' - y)^2$	mean-squared error (MSE)
$\lvert y - y' \rvert$	mean absolute deviation (MAD)
$\mathbb{1}(y \neq y')$	Hamming error/0-1 Loss

Empirical Risk Minimization

$$\widehat{f} = \arg\min_{f \in \mathcal{F}} \widehat{R}(f) = \arg\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i)$$

$\mathcal{F}$: function/model class–how do we model data?

lots of choices. But first: concepts notation.

Training Risk vs. Test Risk

Learning with empirical risk is based on **training risk**: computed on data used in fitting/learning/training/estimating the model.

We are more interested in **test risk** computed on *unseen data*.

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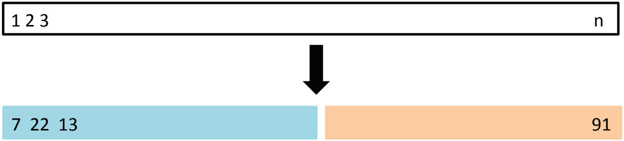
Training Risk vs. Test Risk

Learning with empirical risk is based on **training risk**: computed on data used in fitting/learning/training/estimating the model.

We are more interested in **test risk** computed on *unseen data*. What if we don't have other data?

We can randomly split our data into a test set and a training set.



Help avoid over-fitting to training data min: Let S be a set of ordered values (e.g. numbers)

$$v = \min S$$

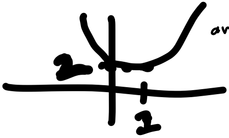
is the largest number such that no number in S is smaller than v

Let $h : \mathcal{X} \mapsto S$ and $X \subset \mathcal{X}$

$$\min_{x \in X} h(x) = \min\{y \mid \exists x \in X \text{ s.t. } y = h(x)\}$$

For $X = \mathcal{X}$

$$\min_{x} h(x) = \min_{x \in \mathcal{X}} h(x)$$



argmin $= \{1\}$
min $= 2$

$$\mathcal{V} = \arg\min_{x} h(x)$$

is the set of all possible values $g \in \mathcal{X}$ such that $h(g) = \min_x h(x)$.

$$g = \arg\min_{x} h(x)$$

for g to be anything in $\mathcal{V}$

Back to learning

Example 0 Suppose $x_i = 1 \ \forall i$ (for all i)

y_i height of person i.

$\mathcal{F} = \{f : \mathbb{R} \mapsto \mathbb{R} \mid \ \forall x \ f(x) = \mu\}$

MSE of $f \equiv \mu$

$$\widehat{R}(\mu) = \frac{1}{n} \sum_{i=1}^{n} (\mu - y_i)^2$$

Solution: $\widehat{\mu} = \frac{1}{n} \sum_i y_i$

Let $\bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_i$

$$
\begin{aligned}
\widehat{R}(\mu) &= \frac{1}{n}\sum_{i=1}^{n}(\mu - y_i)^2 \\
&= \frac{1}{n}\sum_{i=1}^{n}(\mu - \bar{y})^2 + \sum_{i=1}^{n}\frac{1}{n}(\bar{y} - y_i)^2 \quad \text{Let's go through the algebra}
\end{aligned}
$$

Let $\bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_i$

$$\widehat{R}(\mu) = \frac{1}{n}\sum_{i=1}^{n}(\mu - y_i)^2$$

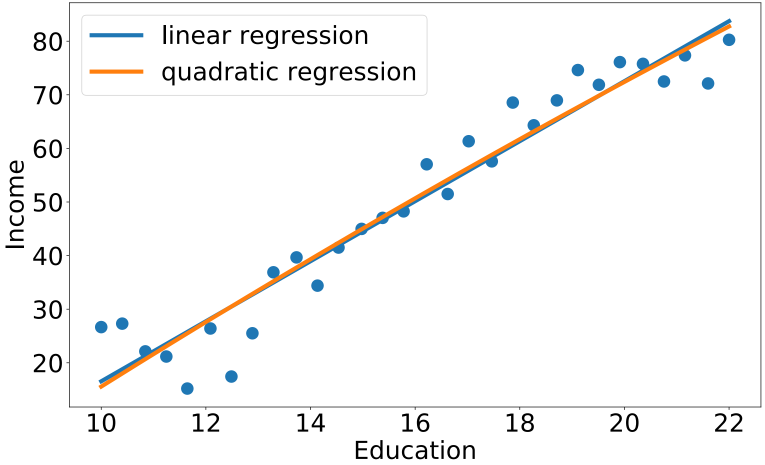
$$= \frac{1}{n}\sum_{i=1}^{n}(\mu - \bar{y})^2 + \frac{1}{n}(\bar{y} - y_i)^2$$ Let's go through the algebra

$$\frac{1}{n}\sum_{i=1}^{n}(\mu - y_i)^2 = \frac{1}{n}\sum_{i=1}^{n}(\mu - \bar{y} + \bar{y} - y_i)^2$$

$$= \frac{1}{n}\sum_{i=1}^{n}(\mu - \bar{y})^2 + \frac{1}{n}\sum_{i=1}^{n}(\bar{y} - y_i)^2 + \frac{2}{n}\sum_{i=1}^{n}(\mu - \bar{y})(\bar{y} - y_i)$$

$$= \frac{1}{n}\sum_{i=1}^{n}(\mu - \bar{y})^2 + \frac{1}{n}\sum_{i=1}^{n}(\bar{y} - y_i)^2$$

Example 1: Linear Regression



Example 1: Linear Regression $\mathcal{X} = \mathbb{R}$ and $\mathcal{Y} = \mathbb{R}$ that is $x_i \in \mathbb{R}$ $y_i \in \mathbb{R}$

Model: $\mathcal{F} = \{f(x) \mid f(x) = \theta_0 + \theta_1 x\} \rightarrow$ linear function

Model: $\mathcal{F} = \{f(x) \mid f(x) = \theta_0 + \theta_1 x + \theta_2 x^2\} \rightarrow$ quadratic function

Note: Generally the first model is considered linear regression, but later we will see why the second model is also linear regression but generally called quadratic regression.

Example 1: Linear Regression

Learn with Ordinary Least Squares. Minimize MSE

$\widehat{f}(x) = \widehat{\theta}_0 + \widehat{\theta}_1 x$

$$\widehat{\theta}_0, \widehat{\theta}_1 \in \arg\min_{\theta_0, \theta_1} \frac{1}{n} \sum_{i=1}^{n} (\theta_0 + \theta_1 x_i - y_i)^2$$

$\widehat{\theta}_0$ is the intercept

$$\widehat{\theta}_1 = \frac{\frac{1}{n}\sum_i (x_i - \bar{x})(y_i - \bar{y})}{\frac{1}{n}\sum_i (x_i - \bar{x})^2}$$

$$\widehat{\theta}_0 = \bar{y} - \widehat{\theta}_1 \bar{x}$$

Can solve this with algebra. We will solve later using derivatives.

Example 2: Linear Regression

Full generality linear regression.

Learn with Ordinary Least Squares. Minimize MSE

$x_i \in \mathbb{R}^d$ (assume that $(x_i)_{(1)} = 1$ for every example)

Take $\theta \in \mathbb{R}^d \to f_\theta(x) = \sum_{j=1}^{d} \theta_{(j)} x_{(j)}$: linear/weighted combination

$$\widehat{\theta} \in \arg\min_{\theta} \frac{1}{n} \sum_{i=1}^{n} (f_\theta(x_i) - y_i)^2$$

Examples

Linear regression in 1-D: Data is $\widetilde{x}_i$ let $x \in \mathbb{R}^2$ $x = (1, \widetilde{x})$

$f(x) = \theta_{(1)} + \theta_{(2)} x_{(2)}$

Exactly the same as Example 1.

Quadratic regression in 1-D: Data is $\widetilde{x}_i$, let $x \in \mathbb{R}^3$ be $x = (1, \widetilde{x}, \widetilde{x}^2)$. This is called a feature mapping.

$$
\begin{aligned}
f(x) &= \theta_1 + \theta_2 x_2 + \theta_3 x_3 \\
&= \theta_1 + \theta_2 \widetilde{x} + \theta_3 \widetilde{x}^2
\end{aligned}
$$

How to find optimal solutions? This is at the heart of ERM based "learning"

Notation

$v, w \in \mathbb{R}^d$, then $\|v\|_2^2 = \sum_{i=1}^d v_{(i)}^2$

$\langle v, w \rangle = \sum_{i=1}^d v_{(i)} w_{(i)}$

Given $y_i \in \mathbb{R}$ for $i \in [n]$, then $y = \mathrm{vec}(y_i) = \text{vector}[y_i] \in \mathbb{R}^n$ with $y_{(i)} = y_i$.

1-D linear regression solutions:

$$\widehat{\theta}_0 = \bar{y} - \widehat{\theta}_1 \bar{x}$$
$$\widehat{\theta}_1 = \frac{\langle \mathrm{vec}(x_i - \bar{x}), \mathrm{vec}(y_i - \bar{y}) \rangle}{\| \mathrm{vec}(x_i - \bar{x}) \|_2^2}$$

Notation

$A \in \mathbb{R}^{n \times d}$ and $X \in \mathbb{R}^{d \times k}$ then $C = AX \in \mathbb{R}^{n \times k}$

$$C_{(ij)} = \sum_{\ell=1}^{d} A_{(i\ell)} X_{(\ell j)}$$

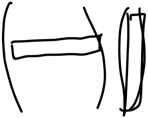
Transpose: $(A^T)_{(ij)} = A_{(ji)}$

Trace: $M \in \mathbb{R}^{d \times d}$ must be square $\mathrm{trace}(M) = \sum_{i=1}^{d} M_{(ii)}$

$C_{(ij)} = \langle A^T_{(i:)}, X_{(:j)} \rangle \quad = \quad A_{(i:)} \cdot X_{(:j)}$

$A_{(i:)}$ is the i^{th} row as a row vector. $X_{(:j)}$ is the j^{th} column as a column vector.

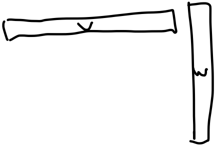
Recall vectors as $d \times 1$ or $1 \times d$ matrices. $v, w \in \mathbb{R}^d$



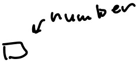
$$(Av)_{(j)} = \sum_{\ell} A_{(i\ell)} v_{(\ell)}$$
$$= \left(A_{(i:)} v\right) = \langle A^T_{(i:)}, v \rangle$$

$$v^T w = \overset{w^T v}{\cancel{w^T v\,\mathrm{quad}}} \quad \text{since transpose of a number is itself}$$
$$= \mathrm{trace}(w^T v) \quad \text{since trace of a number is itself}$$
$$= \mathrm{trace}(v w^T) \quad \text{HW}$$
$$= \langle v, w \rangle$$

$v^T w =$



$=$



Linear regression compactify

$x_i, \theta \in \mathbb{R}^d \to f_\theta(x) = \langle x, \theta \rangle = x^T\theta$

$X = \mathrm{matrix}[x_i]$, $y = \mathrm{vec}(y_i)$

$$X = \begin{pmatrix} - & x_1^T & - \\ - & x_2^T & - \\ & \vdots & \\ - & x_n^T & - \end{pmatrix} \qquad y = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}$$

Ordinary Least Squares

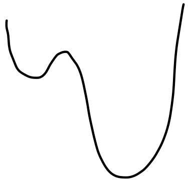
$$\widehat{\theta} \in \arg\min_\theta \frac{1}{n} \sum_{i=1}^{n} (f_\theta(x_i) - y_i)^2$$

Can rewrite empirical risk as

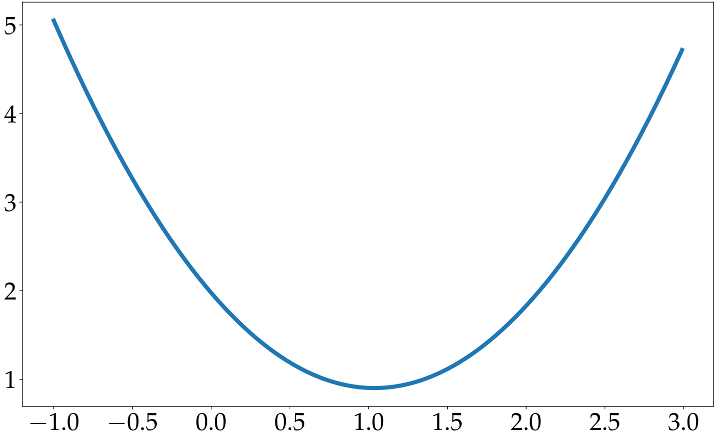
$$\widehat{R}(\theta) = \frac{1}{n} \|X\theta - y\|_2^2$$

Back to optimization

Example 0: $\widehat{R}(\mu) = (\mu - \bar{y})^2 + \frac{1}{n}\sum_{i=1}^{n}(y_i - \bar{y})^2$

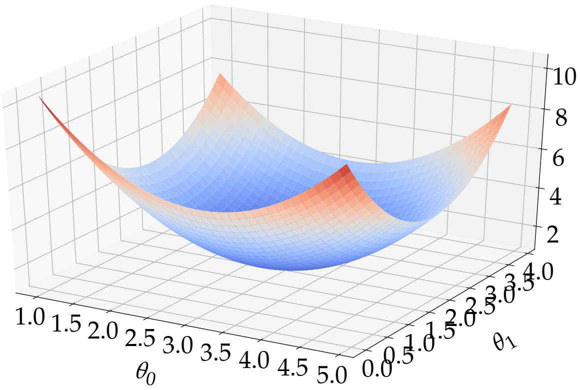


Generated: `y = np.random.randn(100) + 1`



Example 1: $\widehat{R}(\theta_0, \theta_1) = \frac{1}{n}\sum_{i=1}^{n}(\theta_0 + \theta_1 x_i - y_i)^2$

```
n=100;x=np.random.randn(n);
y=x*2+3+np.random.randn(n)
```



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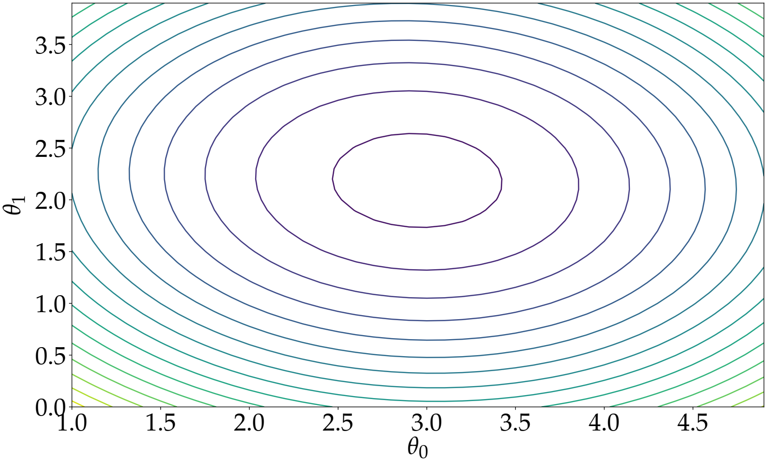
```



Recap

Learning as optimization

$$\widehat{f} = \arg\min_{f \in \mathcal{F}} \widehat{R}(f)$$

$\mathcal{F}$ is a model. So far linear regression.

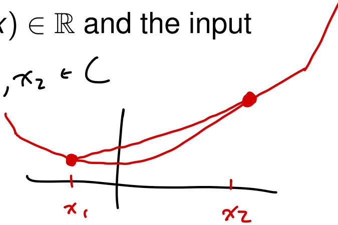
Let's get to solving.

Bowl shapes are special

Notation: Convex functions and gradients

Take $g : C \mapsto \mathbb{R}$ a function $C \subset \mathbb{R}^d$. That is $g(x) \in \mathbb{R}$ and the input space (domain) of g is C.

$x_1, x_2 \in C$



Convex: For $\lambda \in [0, 1]$ we have
$\lambda g(x_1) + (1 - \lambda) g(x_2) \geq g(\lambda x_1 + (1 - \lambda) x_2)$

Partial derivative: Define $e_i \in \mathbb{R}^d$ such that $(e_i)_{(j)} = \mathbb{1}(i = j)$

$$\begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

$$\left.\frac{\partial g(x)}{\partial x_{(i)}}\right|_{x=z} = \lim_{h \to 0} \frac{g(z + h e_i) - g(z)}{h}$$

Partial derivative evaluated at point z.

Overload notation

$$\frac{\partial g(x)}{\partial x_{(i)}}$$

Is partial derivative evaluated at point x

Gradient (local direction of ascent):

$$\nabla_x g(x) = \begin{pmatrix} \frac{\partial g(x)}{\partial x_{(1)}} \\ \frac{\partial g(x)}{\partial x_{(2)}} \\ \vdots \\ \frac{\partial g(x)}{\partial x_{(d)}} \end{pmatrix}$$

Optimization: $\widehat{x} \in \arg\min_x g(x) \iff \nabla g(\widehat{x}) = 0$

For convex: local stationarity implies optimality. Not so for general functions.

Example 0

$$\widehat{R}(\mu) = \frac{1}{n}\sum_{i=1}^{n}(\mu - y_i)^2$$

Take derivative (since no need for partial derivative)

$$\widehat{R}'(\mu) = \frac{2}{n}\sum_{i=1}^{n}(\mu - y_i)$$

Set to zero and solve

$$\frac{2}{n}\sum_{i=1}^{n}(\mu - y_i) = 0$$

$$\widehat{\mu} = \frac{1}{n}\sum_{i=1}^{n} y_i$$

Example 2

$g(\theta) = (x\theta - y)^2$

$g'(\theta) = 2(x\theta - y)x$

$$\widehat{R}(\theta) = \frac{1}{n}\|X\theta - y\|_2^2$$

$e = X\theta - y$

Gradient

$$\nabla\widehat{R}(\theta) = \frac{2}{n}X^T(X\theta - y) \Rightarrow (\nabla\hat{R}(\theta))_{(j)} = (X_{(:,j)})^T e$$

Chain rule, analogous to taking derivative $(x\theta - y)^2$ for $x, y \in \mathbb{R}$. Set to zero.

$$\frac{2}{n}X^T(X\theta - y) = 0$$

Solve

$$\widehat{\theta} = (X^T X)^{-1}X^T y$$

Calculations

$$X = \begin{pmatrix} - x_1^T - \\ - x_2^T - \\ \vdots \\ - x_n^T - \end{pmatrix}$$

$\widehat{R}(\theta) = \frac{1}{n} \sum_{i=1}^{n} (x_i^T \theta - y_i)^2$

$X_{(ij)} = (x_i)_{(j)}$

$$\frac{\partial \widehat{R}}{\partial \theta_{(j)}} = \frac{1}{n} \sum_{i=1}^{n} \frac{\partial (x_i^T \theta - y_i)^2}{\partial \theta_{(j)}}$$

$$= \frac{2}{n} \sum_{i=1}^{n} (x_i)_{(j)} (x_i^T \theta - y_i) \qquad (*)$$

$$= \frac{2}{n} X_{(:j)}^T (X\theta - y)$$

$e = X\theta - y$

$v = X_{(:j)}$

Why?

Define $v \in \mathbb{R}^n$ with $v_{(i)} = (x_i)_{(j)}$

$e \in \mathbb{R}^n$ $\quad e_{(i)} = x_i^T \theta - y_i$

$(*) = \frac{2}{n} v^T e = \frac{2}{n} (X_{(:j)})^T (X\theta - y)$

Matrix Calculations

Notation: $e = X\theta - y$

$\uparrow$ error vector

$$\widehat{R}(\theta) = \|X\theta - y\|_2^2$$

Suppose we have a function $g : \mathbb{R}^n \mapsto \mathbb{R}$, let $h(v) = \nabla g(v)$ then

$$\nabla_\theta g(X\theta - y) = X^T h(v) \quad \text{chain rule}$$

$v = X\theta - y$

Often write

$$\frac{\partial g(X\theta - y)}{\partial(X\theta - y)} = \nabla g(v)|_{v = X\theta - y} = h(X\theta - y)$$

Example: $\cancel{h}\,g(v) = \|v\|_2^2$ can verify that $\nabla \|v\|_2^2 = 2v$, then

$$\nabla \|X\theta - y\|_2^2 = X^T(2(X\theta - y))$$

$$g(v) = \sum_{i=1}^{n} v_{(i)}^2$$

$$\frac{\partial g}{\partial v_{(j)}} = \sum_{i=1}^{n} \frac{\partial (v_{(i)}^2)}{\partial v_{(j)}}$$

$$= \sum_{i=1}^{n} 2 v_{(i)} \mathbb{1}(i=j)$$

$$= 2 v_{(j)}$$

$$\Rightarrow \nabla g = 2v$$

$$\widehat{\theta} = (X^T X)^{-1} X^T y$$

Some issues

- $(X^T X)$ invertibility
- $O(p^3)$ computation (O is like “order of”)
- can be sensitive to noise/outliers

Conclusion

Learning/training/estimating model as optimization

Training vs test set

Data is random, avoid over-fitting to training data

Gradients help to understand optimality