§2. SUPERVISED LEARNING SETUP & LINEAR REGRESSION

06.04

OUTLINE

① choose hypothesis ② choose cost fx

- linear regression + ℓ_2 loss (= OLS).
- Batch/stochastic gradient descent.
- Normal equation. ③ parameter learning/optimization.

→ 3 fundamental building blocks of a (parametric) supervised learning algorithm.

SUPERVISED LEARNING / REGRESSION

⟨Ex⟩ Housing price prediction:

	x_1 size (ft²)	x_2 # bedrooms	x_j …	y price (\$1000s)
$(x^{(1)}, y^{(1)})$	2104	3		400
$(x^{(2)}, y^{(2)})$	1600	3	…	330
$(x^{(3)}, y^{(3)})$	2400	3		369
	⋮	⋮		⋮

Process of supervised learning:

training set
↓
learning algorithm
↓
unseen x → hypothesis h → predicted y

Notation:

- x : input variable / features
- y : output variable / target variable
- (x, y) : 1 training example
- $(x^{(i)}, y^{(i)})$: i-th training example.
- m : # training examples.
- $\{(x^{(i)}, y^{(i)}); i=1,\dots,m\}$: training set.
- x_j : j-th feature.
- n : # features.

$x_j^{(i)}$: (i) index into training examples, $i = 1, \dots, m$. j index into features, $j = (0), 1, \dots, n$.

(eg) $x_1^{(1)} = 2104$
$x_1^{(2)} = 1600$.

LINEAR REGRESSION

— still one of the most widely used algorithms.

How to represent h? ⇒ one of the simplest models: linear regression.

$h_\theta(x) = \theta_0 + \theta_1 x_1 + \cdots + \theta_n x_n$, θ_j: parameter. → Technically: Affine function (linear function + intercept / translation).

↳ shorthand: $h(x)$.

To simplify notation, define dummy feature $x_0 \equiv 1$.

$$\Rightarrow \boxed{h_\theta(x) = \sum_{j=0}^{n} \theta_j x_j = \theta^T x},$$ where $\theta, x \in \mathbb{R}^{n+1}$ (zero-indexed).

Notes.

- Linear regression ⇒ linear in parameters.
  (eg) $h(x) = \theta_0 + \theta_1 \underbrace{x}_{x_1} + \theta_2 \underbrace{x^2}_{x_2}$ ⇒ linear model (V).
- (Univariate) linear regression: $y \in$ scalar / Simple linear regression: $x \in$ scalar. \ Multiple linear regression: $x \in$ vector.
  Multivariate linear regression: $y \in$ vector.

SQUARED ERROR COST FUNCTION

How to choose "good" θ values? ⇒ As a first attempt: choose θ s.t. $h(x) \approx y$ for training examples.
(best E_{in} ≠ best E_{out}.)

Define quantitative measure of model performance:

- loss function : how bad $h(x)$ is doing on 1 example.

⇒ choose ℓ_2 loss: $\boxed{\ell(h_\theta(x), y) = \frac{1}{2}(h_\theta(x) - y)^2}$.

↳ convention (∵ derivatives of ℓ_2).

- Cost function: how bad $h(x)$ is doing on $\underline{m}$ examples.

⇒ Squared error cost function:

$$\boxed{J(\theta) = \frac{1}{2}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2} \Rightarrow \min_\theta J(\theta).$$

↳ is including normalization factor $\frac{1}{m}$ ⇒ mean squared error (MSE) (same optimum).

Notes:

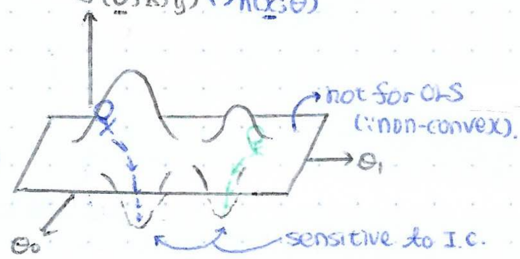
- linear regression + MSE = ordinary least squares (OLS).
- Why ℓ_2? ⇒ There are other forms of loss (eg. ℓ_1 loss $|h_\theta(x) - y|$), but ℓ_2 is a common choice for regression problems:
  - ↳ works well.
  - ↳ math convenience (continuously differentiable).
  - ↳ follows naturally from $y^{(i)} \sim$ i.i.d. Gaussian noise + MLE (special case of GLMs).

GRADIENT DESCENT

How to minimize $J(\theta)$? ⇒ A common search algorithm for a differentiable objective function is gradient descent.

Idea:

- Start w. some initial θ (eg. zero/random initialization).
- keep changing θ at the direction of the steepest descent ($\vec{\nabla} J(\theta)$) to reduce $J(\theta)$, until we hopefully end up at a minimum.
  - ↳ may not converge.
  - ↳ may converge to local min/max, saddle point.



Algorithm:

repeat until convergence {
$$\theta_j := \theta_j - \alpha \frac{\partial J(\theta)}{\partial \theta_j}, \text{ for } j = 0, \dots, 1.$$
}

→ simultaneous update.

assignment ($a := a+1$, ✓) <> truth assertion ($a = a+1$, ✗).

α: learning rate $\in \mathbb{R}^+$.

OR $\theta := \theta - \alpha \vec{\nabla}_\theta J(\theta)$.

For OLS:

Consider 1 example (∵ linearity of differentiation):

$$\frac{\partial J(\theta)}{\partial \theta_j} = \frac{\partial}{\partial \theta_j}\left(\frac{1}{2}(h_\theta(x) - y)^2\right) = \frac{1}{\cancel{2}} \cdot \cancel{2} \cdot (h_\theta(x) - y) \cdot \frac{\partial}{\partial \theta_j}(h_\theta(x) - y)$$
$$= (h_\theta(x) - y) \cdot \frac{\partial}{\partial \theta_j}(\theta_0 x_0 + \dots + \theta_j x_j + \dots + \theta_n x_n - y)$$
$$= (h_\theta(x) - y) \cdot x_j.$$

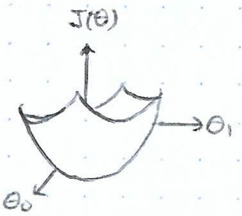
⇒ Least mean squares (LMS) update rule: (OLS + GD.)

repeat until convergence {
$$\theta_j := \theta_j - \alpha \sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)}, \forall j.$$
}

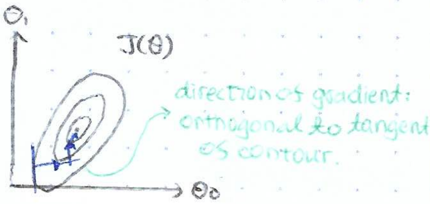
$$\cancel{\underset{(n,1)}{\theta} := \theta - \frac{\alpha}{m} \underset{(n,m)}{X^T} \underset{(m,1)}{(\vec{h} - \vec{y})}}$$

$$\cancel{\begin{bmatrix} | & & | \\ x^{(1)} & \cdots & x^{(m)} \\ | & & | \end{bmatrix} \begin{bmatrix} h(x^{(1)}) - y^{(1)} \\ \vdots \\ h(x^{(m)}) - y^{(m)} \end{bmatrix}}$$

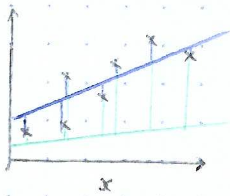
For OLS, $J(\theta)$ is a convex / quadratic fx $\Rightarrow$ 1 global min.



3D surface: bowl-shaped



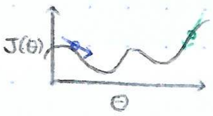
Contours: ellipses.



$\min_\theta J(\theta)$: find optimal θ that leads to the smallest sum of (vertical distance)^2.

Properties

- Minus sign:



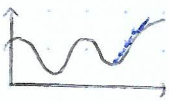
Slope < 0 $\Rightarrow$ move right.
slope > 0 $\Rightarrow$ move left.

For maximization $\Rightarrow$ Gradient ascent:
$$\theta := \theta + \alpha \vec{\nabla} J(\theta).$$

- Local search:

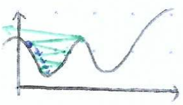
Depending on initialization, may end up at different local minimum
(or wherever $\vec{\nabla} J(\theta) = \vec{0}$)

- Adaptive stepsize:



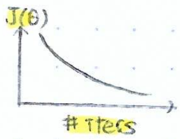
When approaching min, $|\vec{\nabla} J(\theta)| \searrow$, automatically take smaller steps.
$\Rightarrow$ GD can converge w. a fixed α.

- Learning rate:



α too small: take babysteps $\Rightarrow$ slow convergence.
α too large: overshoot minimum $\Rightarrow$ may converge slowly, fail to converge, or even diverge.

Convergence tests:
(1) Check if $\theta^{(t+1)}$ differs significantly from $\theta^{(t)}$
(2) Monitor $J(\theta)$ as a fx of # iters: $\longleftarrow$ much more common.



- Try a few α values on exponential scale, see which value drives $J(\theta)$ down faster.
- $\because$ For sufficiently small α, $J(\theta)$ decreases on every iteration (monotonic convergence)
$\Rightarrow$ If $J(\theta)$ ever increases, use a smaller α.

BGD vs SGD

The algorithm introduced above is called "batch gradient descent (BGD)". ($\sum_{i=1}^{m}$)
$\because$ It scans through the entire training set to take a single step $\Rightarrow$ slow for big data.

Alternative: Stochastic / incremental gradient descent (SGD).

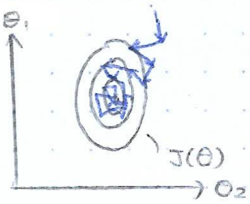
$$\boxed{\begin{array}{l} \text{repeat until convergence} \{ \\ \quad \text{For } i = 1, \dots, m \{ \\ \qquad \theta_j := \theta_j - \alpha \dfrac{\partial J^{(i)}(\theta)}{\partial \theta_j}, \ \forall j \\ \quad \} \\ \} \end{array}}$$

cost / loss for 1 example:
(eg) $J^{(i)}(\theta) = \frac{1}{2}(h_\theta(x^{(i)}) - y^{(i)})^2$

(+) Computationally cheaper per step in comparison to BGD. $\rightarrow$ but also lose the benefit of vectorization.

⇒ When m is large, SGD is used much often than BGD in practice.
↪ $> 10^2, 10^3$

(−): Every step: optimize Θ to fit a particular training example
⇒ noisy trajectory moves towards true minimum on average,
but oscillates around it & is never converged. ↪ tho may be "close enough".



To mitigate the problem ⇒ reduce α over iterations. (cooling schedule)
s.t. the amplitude of oscillations ↘. → (−) one more param to worry about.

Alternatively, one can use an intermediate algorithm "mini-batch GD".

NORMAL EQUATION

→ Normal eqns for nonlinear least squares ⇒ iterative solution — still ls

While GD is a general, iterative search algorithm,
in the case of OLS, it's possible to get the optimal Θ in one step using a closed-form, analytic solution.
↪ In reality, computation of inverse matrix often involves an iterative algorithm (eg eigendecomposition, cholesky algorithm).

Notation for matrix derivatives — to simplify derivation.

Gradient: scalar-by-vector derivative.

$$\nabla_\Theta J(\Theta) = \begin{bmatrix} \frac{\partial J}{\partial \Theta_0} \\ \vdots \\ \frac{\partial J}{\partial \Theta_n} \end{bmatrix} \in \mathbb{R}^{n+1}$$

Scalar-by-matrix derivative: generalization of gradient (but no special name).

for $A \in \mathbb{R}^{m\times n}$, $f(A): \mathbb{R}^{m\times n} \mapsto \mathbb{R}$,

$$\nabla_A f(A) = \begin{bmatrix} \frac{\partial f}{\partial A_{11}} & \cdots & \frac{\partial f}{\partial A_{1n}} \\ \vdots & & \\ \frac{\partial f}{\partial A_{m1}} & \cdots & \frac{\partial f}{\partial A_{mn}} \end{bmatrix} \in \mathbb{R}^{m\times n}$$

↪ collection of elementwise partial derivatives (same shape).

(eg) $A = \begin{bmatrix} 5 & 6 \\ 7 & 8 \end{bmatrix}$, $f(A) = A_{11} + A_{12}^2$.

$$\Rightarrow \nabla_A f(A) = \begin{bmatrix} 1 & 2A_{12} \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 12 \\ 0 & 0 \end{bmatrix}.$$

Tr & properties

If $A \in \mathbb{R}^{n\times n}$ (square matrix), $\mathrm{Tr}(A) = \sum_{i=1}^{n} A_{ii}$.

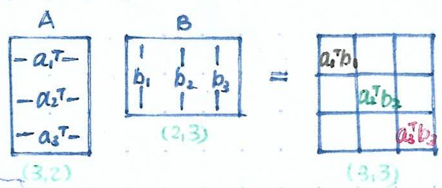
① $\mathrm{Tr}\,A = \mathrm{Tr}\,A^T$. → ∵ flipping A doesn't change the diagonal elements.

② $\nabla_A \mathrm{Tr}\,AB = B^T$. → (cf) $\frac{d(ab)}{da} = b$ (+ match dim).
(m,n)(n,m) (m,n) ✓.
f(A); B: fixed param.

③ Invariant under cyclic permutations →

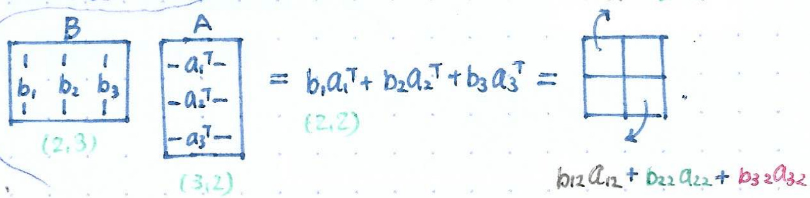
$\mathrm{Tr}\,AB = \mathrm{Tr}\,BA$
(m,n)(n,m) (n,m)(m,n)

$\mathrm{Tr}\,ABC = \mathrm{Tr}\,BCA = \mathrm{Tr}\,CAB$



distribute element multiplication in different ways ⇒ same Tr.

④ $\nabla_A \mathrm{Tr}\,AA^TC = CA + C^TA$. →(cf.) $\frac{d(a^2c)}{da} = 2ac$.
f(A) (m,m)(m,n) (m,m)(m,n) → ✓
(m,n)(n,m)(m,m)



Proof

• Step 1: Express $J(\Theta)$ in array notation.

Define:

"design matrix" $\boxed{X = \begin{bmatrix} -x^{(1)T}- \\ \vdots \\ -x^{(m)T}- \end{bmatrix} \in \mathbb{R}^{m\times(n+1)}}$ & $\vec{y} = \begin{bmatrix} y^{(1)} \\ \vdots \\ y^{(m)} \end{bmatrix} \in \mathbb{R}^{m}$.

$$\Rightarrow X\theta = \begin{bmatrix} -x^{(1)T}- \\ \vdots \\ -x^{(m)T}- \end{bmatrix}\theta = \begin{bmatrix} x^{(1)T}\theta \\ \vdots \\ x^{(m)T}\theta \end{bmatrix} = \begin{bmatrix} h_\theta(x^{(1)}) \\ \vdots \\ h_\theta(x^{(m)}) \end{bmatrix} \in \mathbb{R}^{m}.$$

For scalar s: $s^T = s$.

$$\Rightarrow J(\theta) = \frac{1}{2}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2$$

For vector v: $|v|^2 = \sum_i v_i^2 = v^T v$.

$$= \frac{1}{2}(X\theta - \vec{y})^T(X\theta - \vec{y}) \in \mathbb{R}.$$

• Step 2: Compute $\nabla_\theta J(\theta)$ using Tr properties & set to zero.
└ ∵ $J(\theta)$ is convex ⇒ global min.

$$\nabla_\theta J(\theta) = \nabla_\theta \frac{1}{2}(X\theta - \vec{y})^T(X\theta - \vec{y})$$

$$= \frac{1}{2}\nabla_\theta(\theta^T X^T X\theta - \vec{y}^T X\theta - \theta^T X^T \vec{y} + \cancel{\vec{y}^T\vec{y}}) \rightarrow 0 \ (\because \text{independent of } \theta).$$

$$= \frac{1}{2}\nabla_\theta \mathrm{Tr}(\theta^T X^T X\theta - \vec{y}^T X\theta - \theta^T X^T \vec{y})$$

↳ $s = \mathrm{Tr}\, s$.

$$= \frac{1}{2}\underbrace{\nabla_\theta \mathrm{Tr}\,\theta^T X^T X\theta}_{a} - \frac{1}{2}\underbrace{\nabla_\theta \mathrm{Tr}\,\vec{y}^T X\theta}_{b} - \frac{1}{2}\underbrace{\nabla_\theta \mathrm{Tr}\,\theta^T X^T \vec{y}}_{c}$$

For ⓐ:

$$\nabla_\theta \mathrm{Tr}\,\theta^T X^T X\theta$$
③
$$= \nabla_\theta \mathrm{Tr}\,\underbrace{\theta}_{A}\underbrace{\theta^T}_{A^T}\underbrace{X^T X}_{C}$$
④
$$= X^T X\theta + X^T X\theta$$
$$= 2X^T X\theta.$$

For ⓑ:

$$\nabla_\theta \mathrm{Tr}\,\vec{y}^T X\theta$$
③
$$= \nabla_\theta \mathrm{Tr}\,\underbrace{\theta}_{A}\,\underbrace{\vec{y}^T X}_{B}$$
②
$$= X^T\vec{y}.$$

For ⓒ:

$$\nabla_\theta \mathrm{Tr}\,\theta^T X^T\vec{y}$$
$(\mathrm{Tr})S = (\mathrm{Tr})S^T$ or ①
$$= \nabla_\theta \mathrm{Tr}\,\vec{y}^T X\theta$$
$$= ⓑ.$$

$$\Rightarrow \nabla_\theta J(\theta) = \boxed{X^T X\theta - X^T\vec{y} \triangleq \vec{0}.}$$ "Normal equation"

$$\Rightarrow \theta = (X^T X)^{-1} X^T \vec{y}.$$

$(n+1,n+1)\ (n+1,m)\ (m,1) \rightarrow (n+1,1)$, V.

Notes

- ∵ Normal eqn involves solving $(X^T X)^{-1} \sim O(n^3)$
  ⇒ For large n, GD is preferred.

- When $(X^T X)$ is non-invertible:
  ① redundant features (linearly dependent).
  ② n is too large for given m (not enough linearly independent examples $x^{(i)}$'s).

⇒ Solutions
- Take pseudo-inverse. } → general.
- add regularization.
- manually clean up correlated features. → for ①.
- remove some features/add more examples → for ②.

* Reasons for non-invertible (X^TX): lecture note, p.10

$X^TX \in \mathbb{R}^{(n+1)\times(n+1)}$.

Rationale for ①: insufficient # linearly independent examples   invertibility ⟷ rank.

$$X^TX = \begin{bmatrix} | & & | \\ x^{(1)} & \cdots & x^{(m)} \\ | & & | \end{bmatrix}\begin{bmatrix} - x^{(1)T} - \\ \vdots \\ - x^{(m)T} - \end{bmatrix} = \underbrace{\underbrace{x^{(1)}x^{(1)T}}_{(n+1,n+1),\ \text{rank } 1} + \cdots + x^{(m)}x^{(m)T}}_{m} \in \mathbb{R}^{(n+1)\times(n+1)}.$$

$\Rightarrow rk(X^TX) \leq \min(n+1, m)$.

Obviously, if $m < (n+1) \Rightarrow rk(X^TX) \leq m < (n+1). \Rightarrow$ rank-deficient.
Intuition: # examples is not enough to decide for all degrees of freedom.
(eg. fit 1000-th order polynomial w. 5 data points).

Furthermore, ∵ only linearly-independent $x^{(i)}$'s contribute to the rank.
∴ even $m \geq (n+1)$, (X^TX) may still be rank-deficient.
⇒ Refined to stricter condition: # linearly independent $x^{(i)}$'s $< (n+1)$ ⇒ non-invertible.

Rationale for ②: linearly correlated features.   invertibility ⟷ det.

$$X^TX = X^T\begin{bmatrix} | & & | \\ f_0 & \cdots & f_n \\ | & & | \end{bmatrix}, \quad f_j = \begin{bmatrix} x_j^{(1)} \\ \vdots \\ x_j^{(m)} \end{bmatrix} \in \mathbb{R}^m.$$

$$= \underbrace{\begin{bmatrix} | & & | \\ \underbrace{(X^Tf_0)}_{(n+1,1)} & \cdots & (X^Tf_n) \\ | & & | \end{bmatrix}}_{(n+1)} \in \mathbb{R}^{(n+1)\times(n+1)}.$$

If f_j's are not linearly independent $\Rightarrow f_j = \sum_k \alpha_k f_k$.
$\Rightarrow X^Tf_j = X^T(\sum_k \alpha_k f_k) = \sum_k \alpha_k (X^Tf_k)$. (linear map preserves scalar multiplication & vector addition)
⇒ (X^Tf_j)'s are not linearly independent.
⇒ Volumn of parallelepiped spanned by column vectors (X^Tf_j)'s $= \det(X^TX) = 0$ ⇒ non-invertible.