香港科技大學
THE HONG KONG
UNIVERSITY OF SCIENCE
AND TECHNOLOGY

COMP 5212
Machine Learning

Math Basics

(Largely adapted from Stanford CS229 Slides)

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Linear Independence

A set of vectors $\{x_1, x_2, \ldots x_n\} \subset \mathbb{R}^m$ is said to be ***(linearly) dependent*** if one vector belonging to the set *can* be represented as a linear combination of the remaining vectors; that is, if

$$x_n = \sum_{i=1}^{n-1} \alpha_i x_i$$

for some scalar values $\alpha_1, \ldots, \alpha_{n-1} \in \mathbb{R}$; otherwise, the vectors are ***(linearly) independent***.

Linear Independence

Example:

$$x_1 = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} \quad x_2 = \begin{bmatrix} 4 \\ 1 \\ 5 \end{bmatrix} \quad x_3 = \begin{bmatrix} 2 \\ -3 \\ -1 \end{bmatrix}$$

are linearly dependent because $x_3 = -2x_1 + x_2$.

Rank of a Matrix

- The ***column rank*** of a matrix $A \in \mathbb{R}^{m \times n}$ is the largest number of columns of A that constitute a linearly independent set.

- The ***row rank*** is the largest number of rows of A that constitute a linearly independent set.

- For any matrix $A \in \mathbb{R}^{m \times n}$, it turns out that the column rank of A is equal to the row rank of A (prove it yourself!), and so both quantities are referred to collectively as the ***rank*** of A, denoted as $\mathrm{rank}(A)$.

Properties of Rank

- For $A \in \mathbb{R}^{m \times n}$, $\mathrm{rank}(A) \leq \min(m, n)$. If $\mathrm{rank}(A) = \min(m, n)$, then A is said to be ***full rank***.

- For $A \in \mathbb{R}^{m \times n}$, $\mathrm{rank}(A) = \mathrm{rank}(A^T)$.

- For $A \in \mathbb{R}^{m \times p}$, $B \in \mathbb{R}^{p \times n}$, $\mathrm{rank}(AB) \leq \min(\mathrm{rank}(A), \mathrm{rank}(B))$.

- For $A, B \in \mathbb{R}^{m \times n}$, $\mathrm{rank}(A + B) \leq \mathrm{rank}(A) + \mathrm{rank}(B)$.

The Inverse of a Square Matrix

- The ***inverse*** of a square matrix $A \in \mathbb{R}^{n\times n}$ is denoted A^{-1}, and is the unique matrix such that
$$A^{-1}A = I = AA^{-1}.$$

- We say that A is ***invertible*** or ***non-singular*** if A^{-1} exists and ***non-invertible*** or ***singular*** otherwise.

- In order for a square matrix A to have an inverse A^{-1}, then A must be full rank.

- Properties (Assuming $A, B \in \mathbb{R}^{n\times n}$ are non-singular):
  - $(A^{-1})^{-1} = A$
  - $(AB)^{-1} = B^{-1}A^{-1}$
  - $(A^{-1})^T = (A^T)^{-1}$. For this reason this matrix is often denoted A^{-T}.

Orthogonal Matrices

- Two vectors $x, y \in \mathbb{R}^n$ are ***orthogonal*** if $x^T y = 0$.
- A vector $x \in \mathbb{R}^n$ is ***normalized*** if $\|x\|_2 = 1$.
- A square matrix $U \in \mathbb{R}^{n \times n}$ is ***orthogonal*** if all its columns are orthogonal to each other and are normalized (the columns are then referred to as being ***orthonormal***).

- **Properties:**
  - The inverse of an orthogonal matrix is its transpose.
  $$U^T U = I = UU^T.$$
  - Operating on a vector with an orthogonal matrix will not change its Euclidean norm, i.e.,
  $$\|Ux\|_2 = \|x\|_2$$
  for any $x \in \mathbb{R}^n$, $U \in \mathbb{R}^{n \times n}$ orthogonal.

Span and Projection

- The ***span*** of a set of vectors $\{x_1, x_2, \dots x_n\}$ is the set of all vectors that can be expressed as a linear combination of $\{x_1, \dots, x_n\}$. That is,

$$\operatorname{span}(\{x_1, \dots x_n\}) = \left\{ v : v = \sum_{i=1}^{n} \alpha_i x_i, \;\; \alpha_i \in \mathbb{R} \right\}.$$

- The ***projection*** of a vector $y \in \mathbb{R}^m$ onto the span of $\{x_1, \dots, x_n\}$ is the vector $v \in \operatorname{span}(\{x_1, \dots x_n\})$, such that v is as close as possible to y, as measured by the Euclidean norm $\|v - y\|_2$.

$$\operatorname{Proj}(y; \{x_1, \dots x_n\}) = \operatorname{argmin}_{v \in \operatorname{span}(\{x_1, \dots, x_n\})} \|y - v\|_2.$$

Range

- The ***range*** or the column space of a matrix $A \in \mathbb{R}^{m \times n}$, denoted $\mathcal{R}(A)$, is the the span of the columns of A. In other words,

$$\mathcal{R}(A) = \{v \in \mathbb{R}^m : v = Ax, x \in \mathbb{R}^n\}.$$

- Assuming A is full rank and $n < m$, the projection of a vector $y \in \mathbb{R}^m$ onto the range of A is given by,

$$\mathrm{Proj}(y; A) = \mathrm{argmin}_{v \in \mathcal{R}(A)} \|v - y\|_2.$$

Null Space

The ***nullspace*** of a matrix $A \in \mathbb{R}^{m \times n}$, denoted $\mathcal{N}(A)$ is the set of all vectors that equal 0 when multiplied by A, i.e.,

$$\mathcal{N}(A) = \{x \in \mathbb{R}^n : Ax = 0\}.$$

Determinant

Let $A \in \mathbb{R}^{n \times n}$, $A_{\setminus i, \setminus j} \in \mathbb{R}^{(n-1)\times(n-1)}$ be the *matrix* that results from deleting the ith row and jth column from A.
The general (recursive) formula for the determinant is

$$
\begin{aligned}
|A| &= \sum_{i=1}^{n} (-1)^{i+j} a_{ij} |A_{\setminus i, \setminus j}| \quad \text{(for any } j \in 1, \ldots, n\text{)} \\
&= \sum_{j=1}^{n} (-1)^{i+j} a_{ij} |A_{\setminus i, \setminus j}| \quad \text{(for any } i \in 1, \ldots, n\text{)}
\end{aligned}
$$

Determinant: Example

However, the equations for determinants of matrices up to size 3×3 are fairly common, and it is good to know them:

$$\begin{aligned}
\left|[a_{11}]\right| &= a_{11} \\
\left|\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}\right| &= a_{11}a_{22} - a_{12}a_{21} \\
\left|\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}\right| &= \begin{array}{l} a_{11}a_{22}a_{33} + a_{12}a_{23}a_{31} + a_{13}a_{21}a_{32} \\ \quad -a_{11}a_{23}a_{32} - a_{12}a_{21}a_{33} - a_{13}a_{22}a_{31} \end{array}
\end{aligned}$$

The Determinant

The ***determinant*** of a square matrix $A \in \mathbb{R}^{n\times n}$, is a function $\det : \mathbb{R}^{n\times n} \to \mathbb{R}$, and is denoted $|A|$ or $\det A$.

Given a matrix

$$\begin{bmatrix} — & a_1^T & — \\ — & a_2^T & — \\ & \vdots & \\ — & a_n^T & — \end{bmatrix},$$

consider the set of points $S \subset \mathbb{R}^n$ as follows:

$$S = \{v \in \mathbb{R}^n : v = \sum_{i=1}^{n} \alpha_i a_i \text{ where } 0 \leq \alpha_i \leq 1, i = 1, \ldots, n\}.$$

The absolute value of the determinant of A is a measure of the "volume" of the set S.

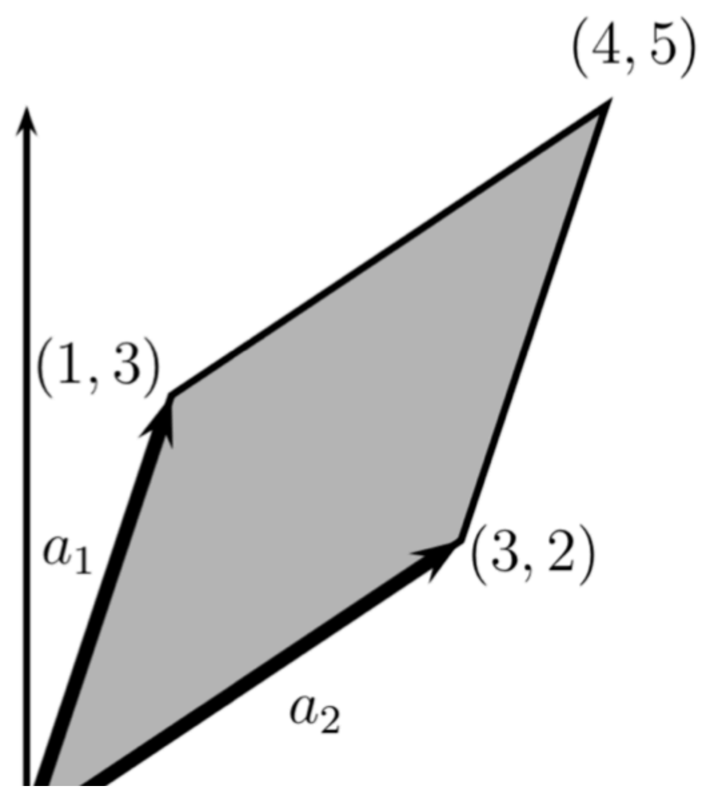
The Determinant

For example, consider the 2×2 matrix,

$$A = \begin{bmatrix} 1 & 3 \\ 3 & 2 \end{bmatrix} \tag{3}$$

Here, the rows of the matrix are

$$a_1 = \begin{bmatrix} 1 \\ 3 \end{bmatrix} \quad a_2 = \begin{bmatrix} 3 \\ 2 \end{bmatrix}$$



The Determinant: Properties

Algebraically, the determinant satisfies the following three properties:

1. The determinant of the identity is 1, $|I| = 1$. (Geometrically, the volume of a unit hypercube is 1).

2. Given a matrix $A \in \mathbb{R}^{n \times n}$, if we multiply a single row in A by a scalar $t \in \mathbb{R}$, then the determinant of the new matrix is $t|A|$, (Geometrically, multiplying one of the sides of the set S by a factor t causes the volume to increase by a factor t.)

3. If we exchange any two rows a_i^T and a_j^T of A, then the determinant of the new matrix is $-|A|$, for example

The Determinant: Properties

- For $A \in \mathbb{R}^{n \times n}$, $|A| = |A^T|$.
- For $A, B \in \mathbb{R}^{n \times n}$, $|AB| = |A||B|$.
- For $A \in \mathbb{R}^{n \times n}$, $|A| = 0$ if and only if A is singular (i.e., non-invertible). (If A is singular then it does not have full rank, and hence its columns are linearly dependent. In this case, the set S corresponds to a "flat sheet" within the n-dimensional space and hence has zero volume.)
- For $A \in \mathbb{R}^{n \times n}$ and A non-singular, $|A^{-1}| = 1/|A|$.

Eigenvalues and Eigenvectors

Given a square matrix $A \in \mathbb{R}^{n \times n}$, we say that $\lambda \in \mathbb{C}$ is an ***eigenvalue*** of A and $x \in \mathbb{C}^n$ is the corresponding ***eigenvector*** if

$$Ax = \lambda x, \quad x \neq 0.$$

Intuitively, this definition means that multiplying A by the vector x results in a new vector that points in the same direction as x, but scaled by a factor λ.

Gradient over Matrix

Suppose that $f : \mathbb{R}^{m\times n} \to \mathbb{R}$ is a function that takes as input a matrix A of size $m \times n$ and returns a real value. Then the ***gradient*** of f (with respect to $A \in \mathbb{R}^{m\times n}$) is the matrix of partial derivatives, defined as:

$$\nabla_A f(A) \in \mathbb{R}^{m\times n} = \begin{bmatrix} \frac{\partial f(A)}{\partial A_{11}} & \frac{\partial f(A)}{\partial A_{12}} & \cdots & \frac{\partial f(A)}{\partial A_{1n}} \\ \frac{\partial f(A)}{\partial A_{21}} & \frac{\partial f(A)}{\partial A_{22}} & \cdots & \frac{\partial f(A)}{\partial A_{2n}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f(A)}{\partial A_{m1}} & \frac{\partial f(A)}{\partial A_{m2}} & \cdots & \frac{\partial f(A)}{\partial A_{mn}} \end{bmatrix}$$

i.e., an $m \times n$ matrix with

$$(\nabla_A f(A))_{ij} = \frac{\partial f(A)}{\partial A_{ij}}.$$

Gradient over Vector

Note that the size of $\nabla_A f(A)$ is always the same as the size of A. So if, in particular, A is just a vector $x \in \mathbb{R}^n$,

$$\nabla_x f(x) = \begin{bmatrix} \frac{\partial f(x)}{\partial x_1} \\ \frac{\partial f(x)}{\partial x_2} \\ \vdots \\ \frac{\partial f(x)}{\partial x_n} \end{bmatrix}.$$

It follows directly from the equivalent properties of partial derivatives that:

- $\nabla_x(f(x) + g(x)) = \nabla_x f(x) + \nabla_x g(x)$.
- For $t \in \mathbb{R}$, $\nabla_x(t\, f(x)) = t\nabla_x f(x)$.

The Hessian

Suppose that $f : \mathbb{R}^n \to \mathbb{R}$ is a function that takes a vector in $\mathbb{R}^n$ and returns a real number. Then the ***Hessian*** matrix with respect to x, written $\nabla_x^2 f(x)$ or simply as H is the $n \times n$ matrix of partial derivatives,

$$\nabla_x^2 f(x) \in \mathbb{R}^{n\times n} = \begin{bmatrix} \frac{\partial^2 f(x)}{\partial x_1^2} & \frac{\partial^2 f(x)}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f(x)}{\partial x_2 \partial x_1} & \frac{\partial^2 f(x)}{\partial x_2^2} & \cdots & \frac{\partial^2 f(x)}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f(x)}{\partial x_n \partial x_1} & \frac{\partial^2 f(x)}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_n^2} \end{bmatrix}.$$

Note that the Hessian is always symmetric, since

$$\frac{\partial^2 f(x)}{\partial x_i \partial x_j} = \frac{\partial^2 f(x)}{\partial x_j \partial x_i}.$$

Gradients of Linear Functions

For $x \in \mathbb{R}^n$, let $f(x) = b^T x$ for some known vector $b \in \mathbb{R}^n$. Then

$$f(x) = \sum_{i=1}^{n} b_i x_i$$

so

$$\frac{\partial f(x)}{\partial x_k} = \frac{\partial}{\partial x_k} \sum_{i=1}^{n} b_i x_i = b_k.$$

From this we can easily see that $\nabla_x b^T x = b$. This should be compared to the analogous situation in single variable calculus, where $\partial/(\partial x)\ ax = a$.

Common Gradient Formula

- $\nabla_x b^T x = b$
- $\nabla_x^2 b^T x = 0$
- $\nabla_x x^T A x = 2Ax$ (if A symmetric)
- $\nabla_x^2 x^T A x = 2A$ (if A symmetric)

Least Squares

- Given a full rank matrix $A \in \mathbb{R}^{m \times n}$, and a vector $b \in \mathbb{R}^m$ such that $b \notin \mathcal{R}(A)$, we want to find a vector x such that Ax is as close as possible to b, as measured by the square of the Euclidean norm $\|Ax - b\|_2^2$.

Outline

- Linear Algebra Review

- Probability Review

Basic Concepts

- Performing an **experiment** $\rightarrow$ **outcome**
- **Sample Space** (S): set of all possible outcomes of an experiment
- **Event** (E): a subset of S ($E \subseteq S$)

- **Probability** (**Bayesian** definition)

  A number between 0 and 1 to which we ascribe meaning
  i.e. our belief that an event E occurs

- **Frequentist** definition of probability

$$P(E) = \lim_{n \to \infty} \frac{n(E)}{n}$$

Axiom 1: $0 \leq P(E) \leq 1$
Axiom 2: $P(S) = 1$

$E \subseteq F$, then $P(E) \leq P(F)$
$P(E \cup F) = P(E) + P(F) - P(EF)$ (Inclusion-Exclusion Principle)

General Inclusion-Exclusion Principle:

$$P\left(\bigcup_{i=1}^{n} E_i\right) = \sum_{r=1}^{n} (-1)^{r+1} \sum_{i_1 < \cdots < i_r} P(E_{i_1} E_{i_2} \ldots E_{i_r})$$

Equally Likely Outcomes: Define S as a sample space with equally likely outcomes. Then
$P(E) = \dfrac{|E|}{|S|}$

Conditional Probability and Bayes' Rule

For any events A, B such that $P(B) \neq 0$, we define:

$$P(A \mid B) := \frac{P(A \cap B)}{P(B)}$$

Let's apply conditional probability to obtain **Bayes' Rule**!

$$P(B \mid A) = \frac{P(B \cap A)}{P(A)} = \frac{P(A \cap B)}{P(A)}$$

$$= \boxed{\frac{P(B)P(A \mid B)}{P(A)}}$$

Conditioned Bayes' Rule: given events A, B, C,

$$P(A \mid B, C) = \frac{P(B \mid A, C)P(A \mid C)}{P(B \mid C)}$$

Law of Total Probability

Let $B_1, \ldots, B_n$ be n disjoint events whose union is the entire sample space. Then, for any event A,

$$\begin{aligned} P(A) &= \sum_{i=1}^{n} P(A \cap B_i) \\ &= \sum_{i=1}^{n} P(A \mid B_i) P(B_i) \end{aligned}$$

We can then write Bayes' Rule as:

$$\begin{aligned} P(B_k \mid A) &= \frac{P(B_k)P(A \mid B_k)}{P(A)} \\ &= \boxed{\frac{P(B_k)P(A \mid B_k)}{\sum_{i=1}^{n} P(A \mid B_i)P(B_i)}} \end{aligned}$$

Chain Rule

For any n events $A_1, \ldots, A_n$, the joint probability can be expressed as a product of conditionals:

$$
\begin{aligned}
&P(A_1 \cap A_2 \cap \ldots \cap A_n) \\
&\quad = P(A_1)P(A_2 \mid A_1)P(A_3 \mid A_2 \cap A_1) \ldots P(A_n \mid A_{n-1} \cap A_{n-2} \cap \ldots \cap A_1)
\end{aligned}
$$

Independence

Events A, B are independent if

$$P(AB) = P(A)P(B)$$

We denote this as $A \perp B$. From this, we know that if $A \perp B$,

$$P(A \mid B) = \frac{P(A \cap B)}{P(B)} = \frac{P(A)P(B)}{P(B)} = P(A)$$

Implication: If two events are independent, observing one event does not change the probability that the other event occurs.

In general: events $A_1, \ldots, A_n$ are **mutually independent** if

$$P(\bigcap_{i \in S} A_i) = \prod_{i \in S} P(A_i)$$

Random Variable

A **random variable** X is a variable that probabilistically takes on different values. It maps outcomes to real values

Probability Mass Function (PMF)

Given a **discrete** RV X, a PMF maps values of X to probabilities.

$$p_X(x) := p(x) := P(X = x)$$

For a valid PMF, $\sum_{x \in Val(x)} p_X(x) = 1$.

Cumulative Distribution Function (CDF)

A CDF maps a continuous RV to a probability (i.e. $\mathbb{R} \to [0,1]$)

$$F_X(a) := F(a) := P(X \leq a)$$

A CDF must fulfill the following:

- $\lim_{x \to -\infty} F_X(x) = 0$
- $\lim_{x \to \infty} F_X(x) = 1$
- If $a \leq b$, then $F_X(a) \leq F_X(b)$ (i.e. CDF must be nondecreasing)

Also note: $P(a \leq X \leq b) = F_X(b) - F_X(a)$.

Probability Density Function (PDF)

PDF of a continuous RV is simply the derivative of the CDF.

$$f_X(x) := f(x) := \frac{dF_X(x)}{dx}$$

Expectation

Let g be an arbitrary real-valued function.

- If X is a discrete RV with PMF p_X:

$$\mathbb{E}[g(X)] := \sum_{x \in Val(X)} g(x) p_X(x)$$

- If X is a continuous RV with PDF f_X:

$$\mathbb{E}[g(X)] := \int_{-\infty}^{\infty} g(x) f_X(x) dx$$

Intuitively, expectation is a weighted average of the values of $g(x)$, weighted by the probability of x.

Conditional Expectation

$\mathbb{E}[X \mid Y] = \sum_{x \in Val(x)} x p_{X|Y}(x|y)$ is a function of Y.

Properties of Expectation

For any constant $a \in \mathbb{R}$ and arbitrary real function f:

- $\mathbb{E}[a] = a$
- $\mathbb{E}[af(X)] = a\mathbb{E}[f(X)]$

Linearity of Expectation

Given n real-valued functions $f_1(X), \ldots, f_n(X)$,

$$\mathbb{E}[\sum_{i=1}^{n} f_i(X)] = \sum_{i=1}^{n} \mathbb{E}[f_i(X)]$$

Example

El Goog sources two batteries, A and B, for its phone. A phone with battery A runs on average 12 hours on a single charge, but only 8 hours on average with battery B. El Goog puts battery A in 80% of its phones and battery B in the rest. If you buy a phone from El Goog, how many hours do you expect it to run on a single charge?

Variance

The **variance** of a RV X measures how concentrated the distribution of X is around its mean.

$$\begin{aligned} Var(X) &:= \mathbb{E}[(X - \mathbb{E}[X])^2] \\ &= \mathbb{E}[X^2] - \mathbb{E}[X]^2 \end{aligned}$$

Interpretation: $Var(X)$ is the expected deviation of X from $\mathbb{E}[X]$.
Properties: For any constant $a \in \mathbb{R}$, real-valued function $f(X)$

- $Var[a] = 0$
- $Var[af(X)] = a^2 Var[f(X)]$

Example Distributions

Distribution	PDF or PMF	Mean	Variance
$Bernoulli(p)$	$\begin{cases} p, & \text{if } x = 1 \\ 1 - p, & \text{if } x = 0. \end{cases}$	p	$p(1-p)$
$Binomial(n, p)$	$\binom{n}{k} p^k (1-p)^{n-k}$ for $k = 0, 1, ..., n$	np	$np(1-p)$
$Geometric(p)$	$p(1-p)^{k-1}$ for $k = 1, 2, \ldots$	$\frac{1}{p}$	$\frac{1-p}{p^2}$
$Poisson(\lambda)$	$\frac{e^{-\lambda}\lambda^k}{k!}$ for $k = 0, 1, \ldots$	λ	λ
$Uniform(a, b)$	$\frac{1}{b-a}$ for all $x \in (a, b)$	$\frac{a+b}{2}$	$\frac{(b-a)^2}{12}$
$Gaussian(\mu, \sigma^2)$	$\frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$ for all $x \in (-\infty, \infty)$	μ	σ^2
$Exponential(\lambda)$	$\lambda e^{-\lambda x}$ for all $x \geq 0, \lambda \geq 0$	$\frac{1}{\lambda}$	$\frac{1}{\lambda^2}$

Joint and Marginal Distributions

- **Joint PMF** for discrete RV's X, Y:

$$p_{XY}(x, y) = P(X = x, Y = y)$$

Note that $\sum_{x \in Val(X)} \sum_{y \in Val(Y)} p_{XY}(x, y) = 1$

- **Marginal PMF** of X, given joint PMF of X, Y:

$$p_X(x) = \sum_y p_{XY}(x, y)$$

Joint and Marginal Distributions

- **Joint PDF** for continuous RV's $X_1, ..., X_n$:

$$f(x_1, ..., x_n) = \frac{\delta^n F(x_1, ...x_n)}{\delta x_1 \delta x_2 ... \delta x_n}$$

Note that $\int_{x_1} \int_{x_2} ... \int_{x_n} f(x_1, ..., x_n) dx_1 ... dx_n = 1$

- **Marginal PDF** of X_1, given joint PDF of $X_1, ..., X_n$:

$$f_{X_1}(x_1) = \int_{x_2} ... \int_{x_n} f(x_1, ..., x_n) dx_2 ... dx_n$$

Expectation for multiple random variables

Given two RV's X, Y and a function $g : \mathbb{R}^2 \to \mathbb{R}$ of X, Y,

- for discrete X, Y:

$$\mathbb{E}[g(X,Y)] := \sum_{x \in Val(x)} \sum_{y \in Val(y)} g(x,y) p_{XY}(x,y)$$

- for continuous X, Y:

$$\mathbb{E}[g(X,Y)] := \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} g(x,y) f_{XY}(x,y) dxdy$$

Covariance

Intuitively: measures how much one RV's value tends to move with another RV's value. For RV's X, Y:

$$
\begin{aligned}
Cov[X, Y] &:= \mathbb{E}\left[(X - \mathbb{E}[X])(Y - \mathbb{E}[Y])\right] \\
&= \mathbb{E}[XY] - \mathbb{E}[X]\mathbb{E}[Y]
\end{aligned}
$$

- If $Cov[X, Y] < 0$, then X and Y are negatively correlated
- If $Cov[X, Y] > 0$, then X and Y are positively correlated
- If $Cov[X, Y] = 0$, then X and Y are uncorrelated

Variance of two variables

$$Var[X + Y] = Var[X] + Var[Y] + 2Cov[X, Y]$$

Conditional distributions for RVs

Works the same way with RV's as with events:

- For discrete X, Y:

$$p_{Y|X}(y|x) = \frac{p_{XY}(x,y)}{p_X(x)}$$

- For continuous X, Y:

$$f_{Y|X}(y|x) = \frac{f_{XY}(x,y)}{f_X(x)}$$

- In general, for continuous $X_1, \ldots, X_n$:

$$f_{X_1|X_2,\ldots,X_n}(x_1|x_2,\ldots,x_n) = \frac{f_{X_1,X_2,\ldots,X_n}(x_1,x_2,\ldots,x_n)}{f_{X_2,\ldots,X_n}(x_2,\ldots,x_n)}$$

Bayes' Rule for RVs

Also works the same way for RV's as with events:

- For discrete X, Y:

$$p_{Y|X}(y|x) = \frac{p_{X|Y}(x|y)p_Y(y)}{\sum_{y' \in Val(Y)} p_{X|Y}(x|y')p_Y(y')}$$

- For continuous X, Y:

$$f_{Y|X}(y|x) = \frac{f_{X|Y}(x|y)f_Y(y)}{\int_{-\infty}^{\infty} f_{X|Y}(x|y')f_Y(y')dy'}$$

Random Vectors

Given n RV's $X_1, \dots, X_n$, we can define a random vector X s.t.

$$X = \begin{bmatrix} X_1 \\ X_2 \\ \vdots \\ X_n \end{bmatrix}$$

Note: all the notions of joint PDF/CDF will apply to X.
Given $g : \mathbb{R}^n \to \mathbb{R}^m$, we have:

$$g(x) = \begin{bmatrix} g_1(x) \\ g_2(x) \\ \vdots \\ g_m(x) \end{bmatrix}, \mathbb{E}[g(X)] = \begin{bmatrix} \mathbb{E}[g_1(X)] \\ \mathbb{E}[g_2(X)] \\ \vdots \\ \mathbb{E}[g_m(X)] \end{bmatrix}$$

Covariance Matrices

For a random vector $X \in \mathbb{R}^n$, we define its **covariance matrix** Σ as the $n \times n$ matrix whose ij-th entry contains the covariance between X_i and X_j.

$$\Sigma = \begin{bmatrix} Cov[X_1, X_1] & \dots & Cov[X_1, X_n] \\ \vdots & \ddots & \vdots \\ Cov[X_n, X_1] & \dots & Cov[X_n, X_n] \end{bmatrix}$$

applying linearity of expectation and the fact that $Cov[X_i, X_j] = \mathbb{E}[(X_i - \mathbb{E}[X_i])(X_j - \mathbb{E}[X_j])]$, we obtain

$$\Sigma = \mathbb{E}[(X - \mathbb{E}[X])(X - \mathbb{E}[X])^T]$$

Properties:

- Σ is symmetric and PSD
- If $X_i \perp X_j$ for all i, j, then $\Sigma = diag(Var[X_1], ..., Var[X_n])$

Multivariate Gaussian

The multivariate Gaussian $X \sim \mathcal{N}(\mu, \Sigma)$, $X \in \mathbb{R}^n$:

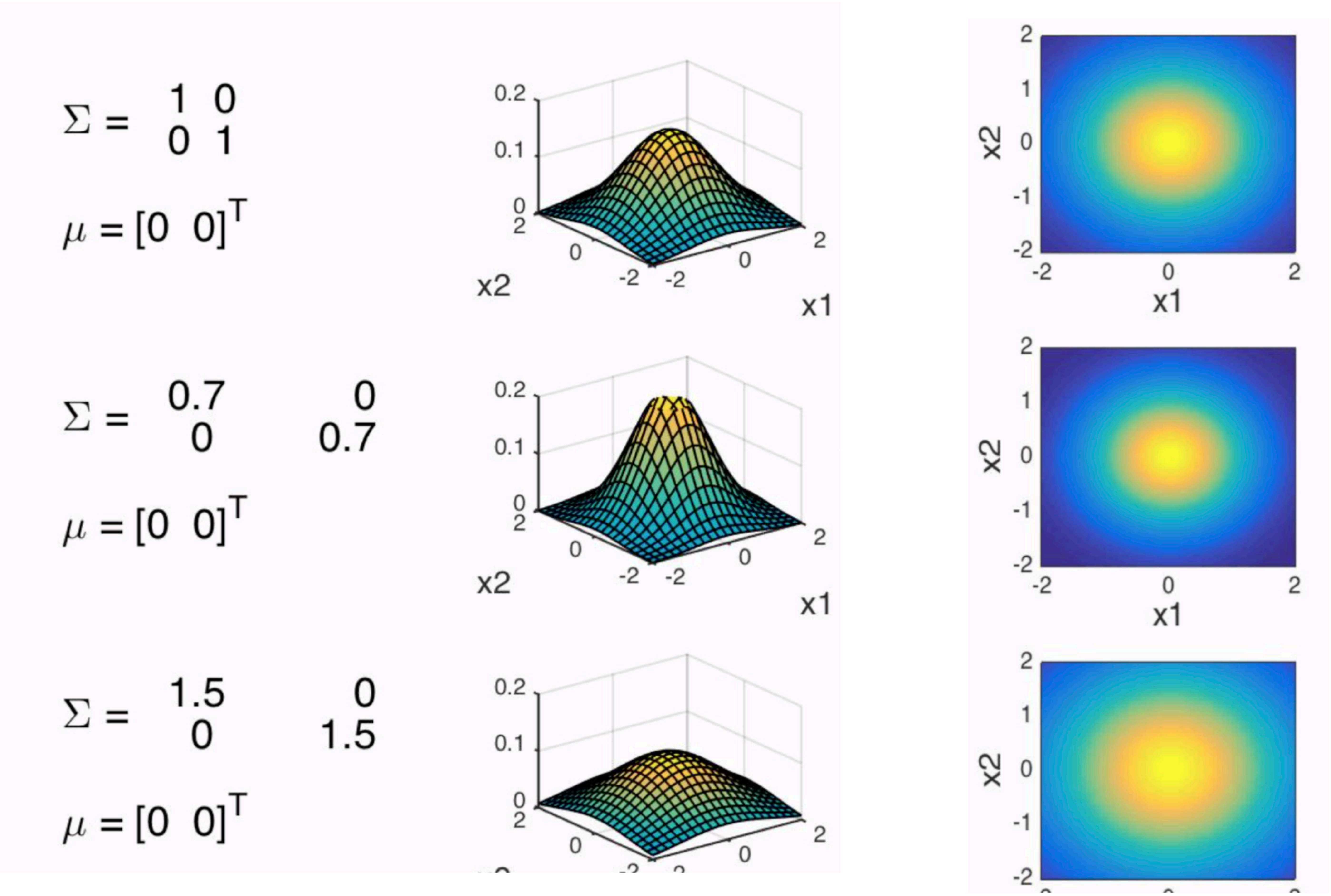
$$p(x; \mu, \Sigma) = \frac{1}{det(\Sigma)^{\frac{1}{2}}(2\pi)^{\frac{n}{2}}} \exp\left(-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)\right)$$

Gaussian when $n = 1$.

$$p(x; \mu, \sigma^2) = \frac{1}{\sigma(2\pi)^{\frac{1}{2}}} \exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2\right)$$

Notice that if $\Sigma \in \mathbb{R}^{1\times 1}$, then $\Sigma = Var[X_1] = \sigma^2$, and so $\Sigma^{-1} = \frac{1}{\sigma^2}$ and $det(\Sigma)^{\frac{1}{2}} = \sigma$

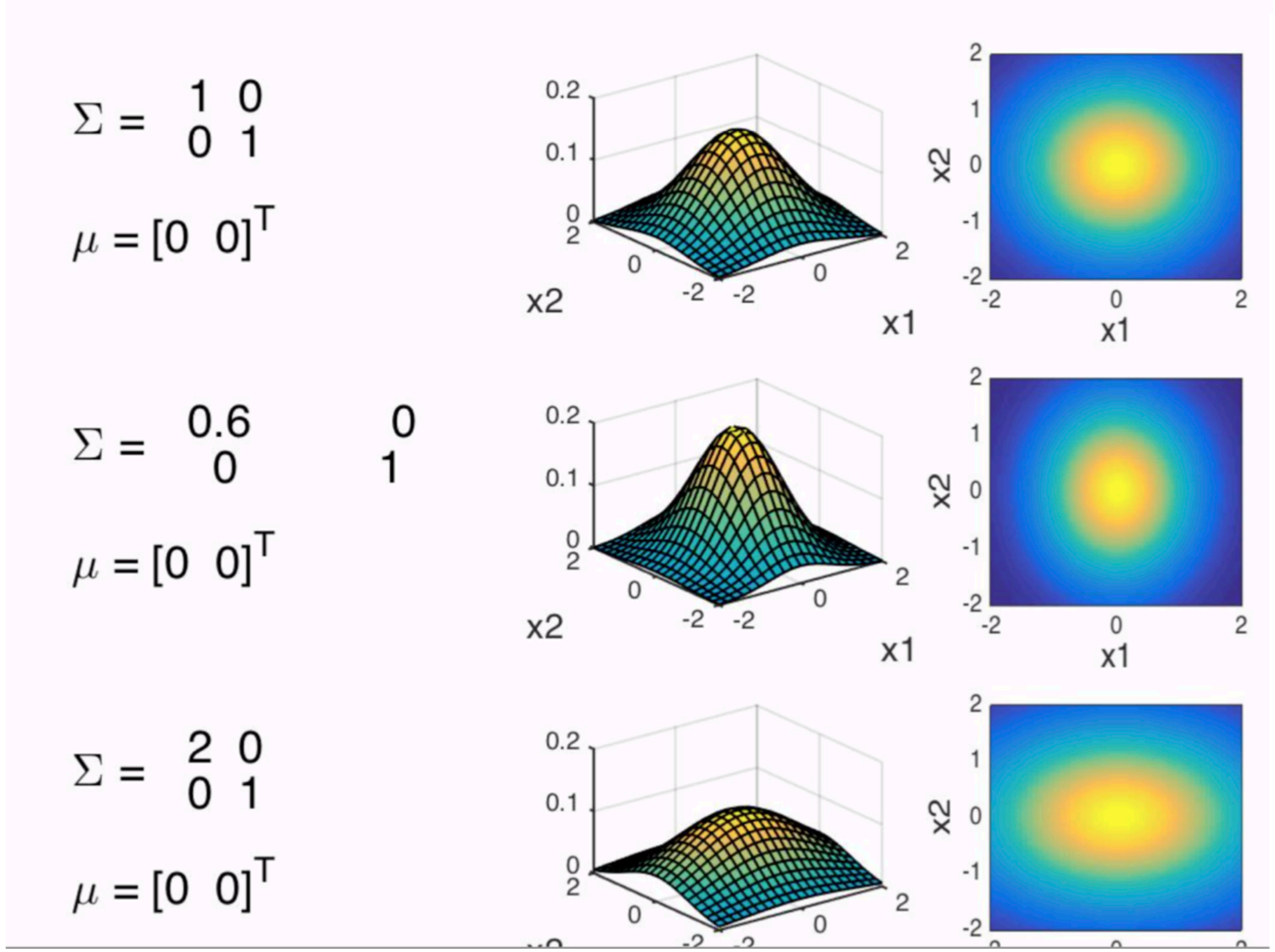
MV Gaussian Visualization



Effect of changing variance

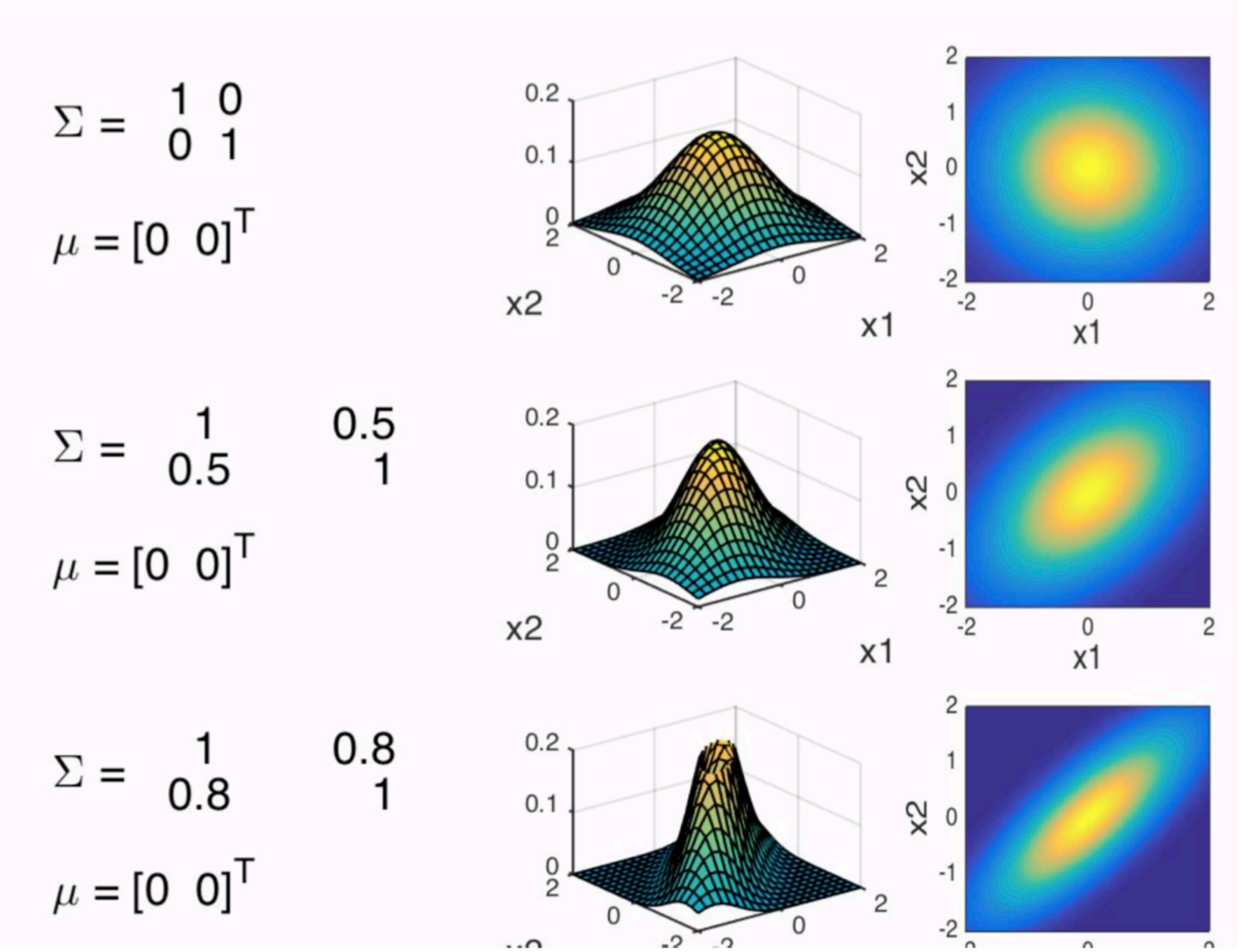
MV Gaussian Visualization

If $Var[X_1] \neq Var[X_2]$:



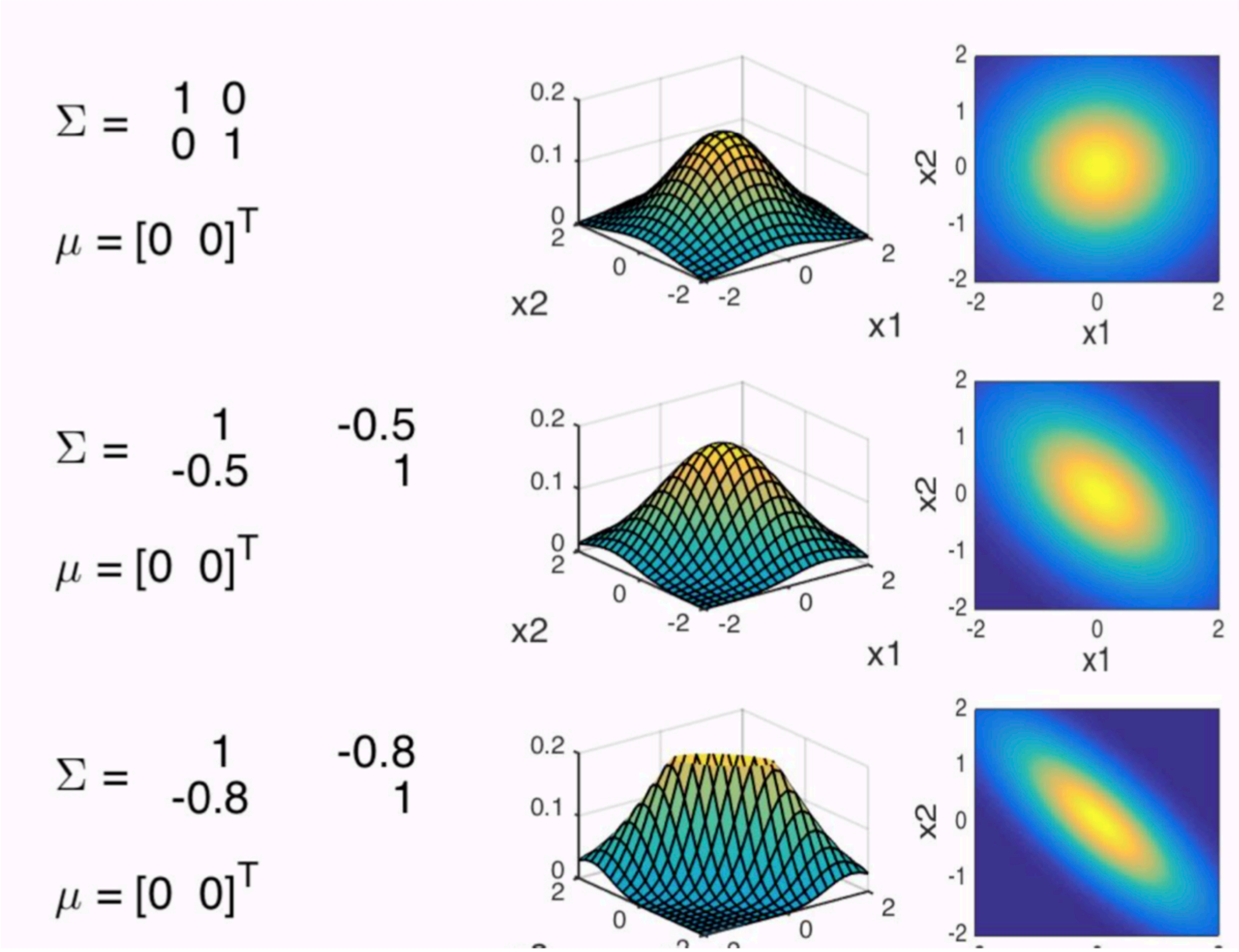
MV Gaussian Visualization

If X_1 and X_2 are positively correlated:



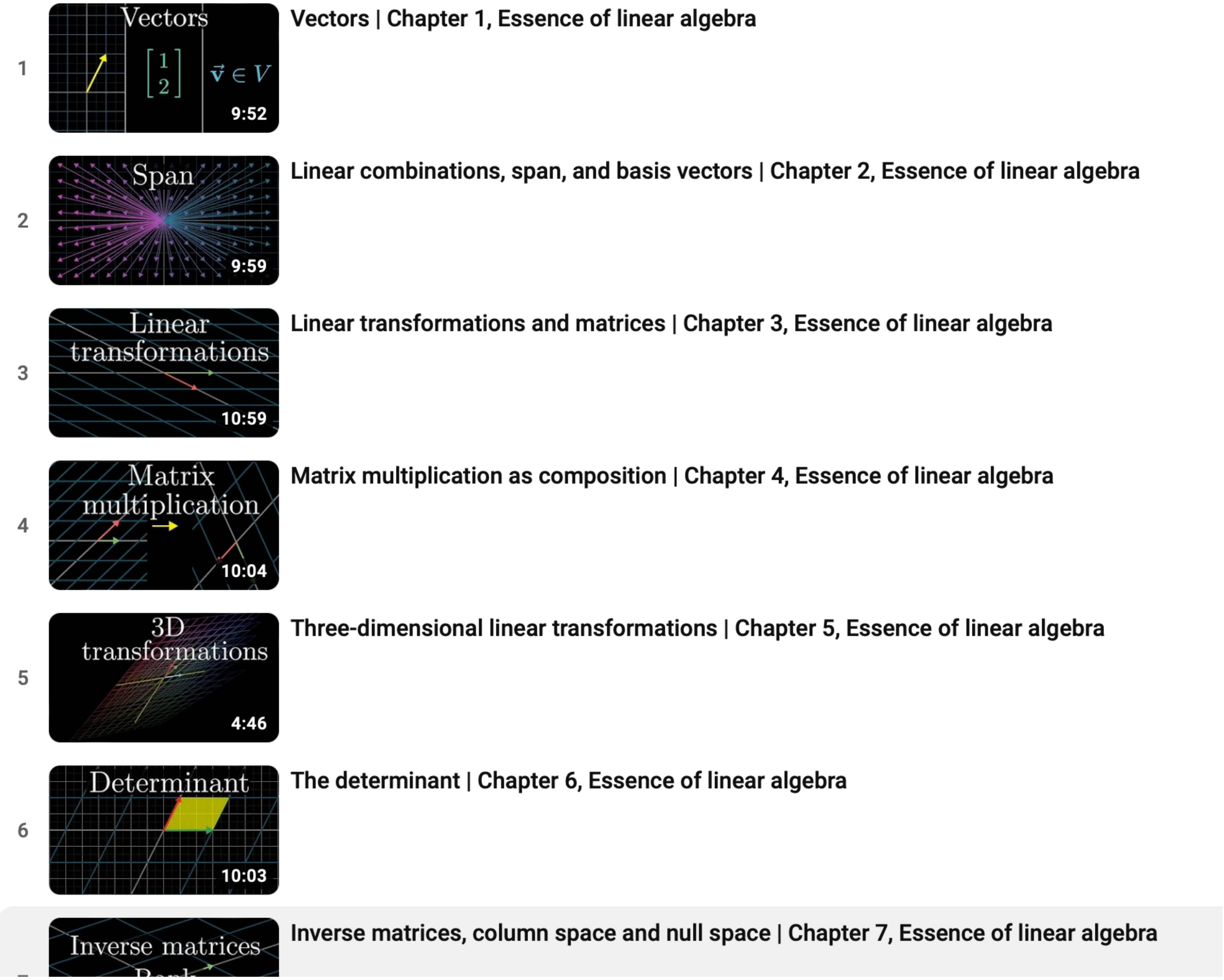
MV Gaussian Visualization

If X_1 and X_2 are negatively correlated:

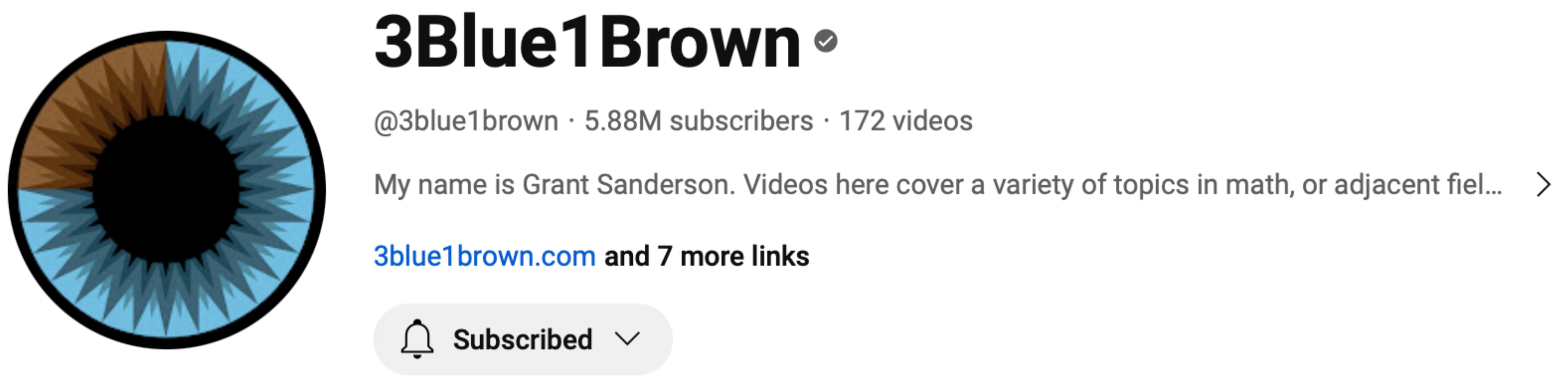


The purpose of computation is insight, not numbers.

- Richard Hamming



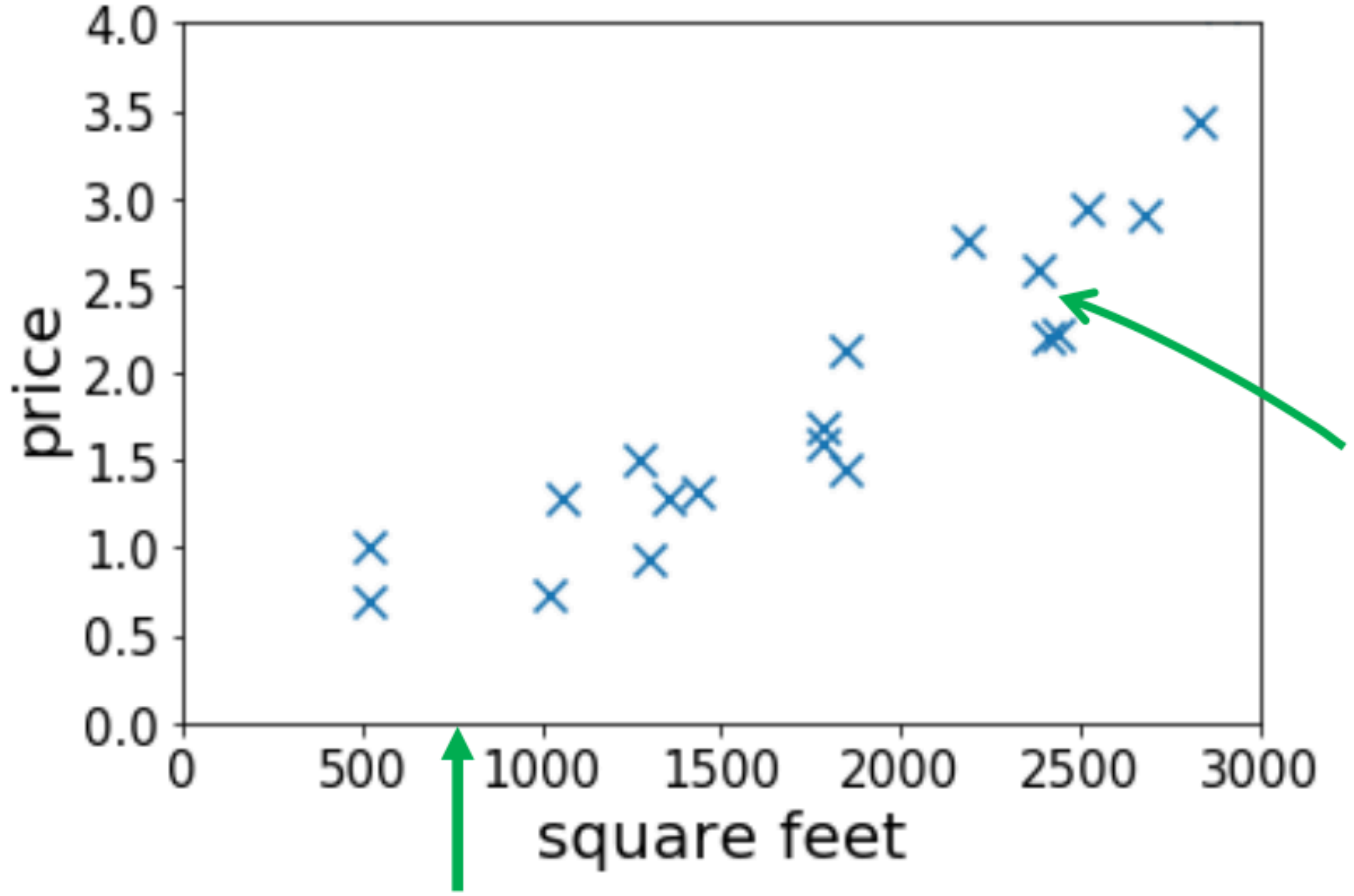
https://www.youtube.com/@3blue1brown/courses



Supervised Learning: Regression

Supervised Learning

- A hypothesis or a prediction function is function $h : \mathcal{X} \to \mathcal{Y}$



15th sample
$(x^{(15)}, y^{(15)})$

$x = 800$
$y = ?$

X

CAT Y

Supervised Learning

- A hypothesis or a prediction function is function $h : \mathcal{X} \to \mathcal{Y}$

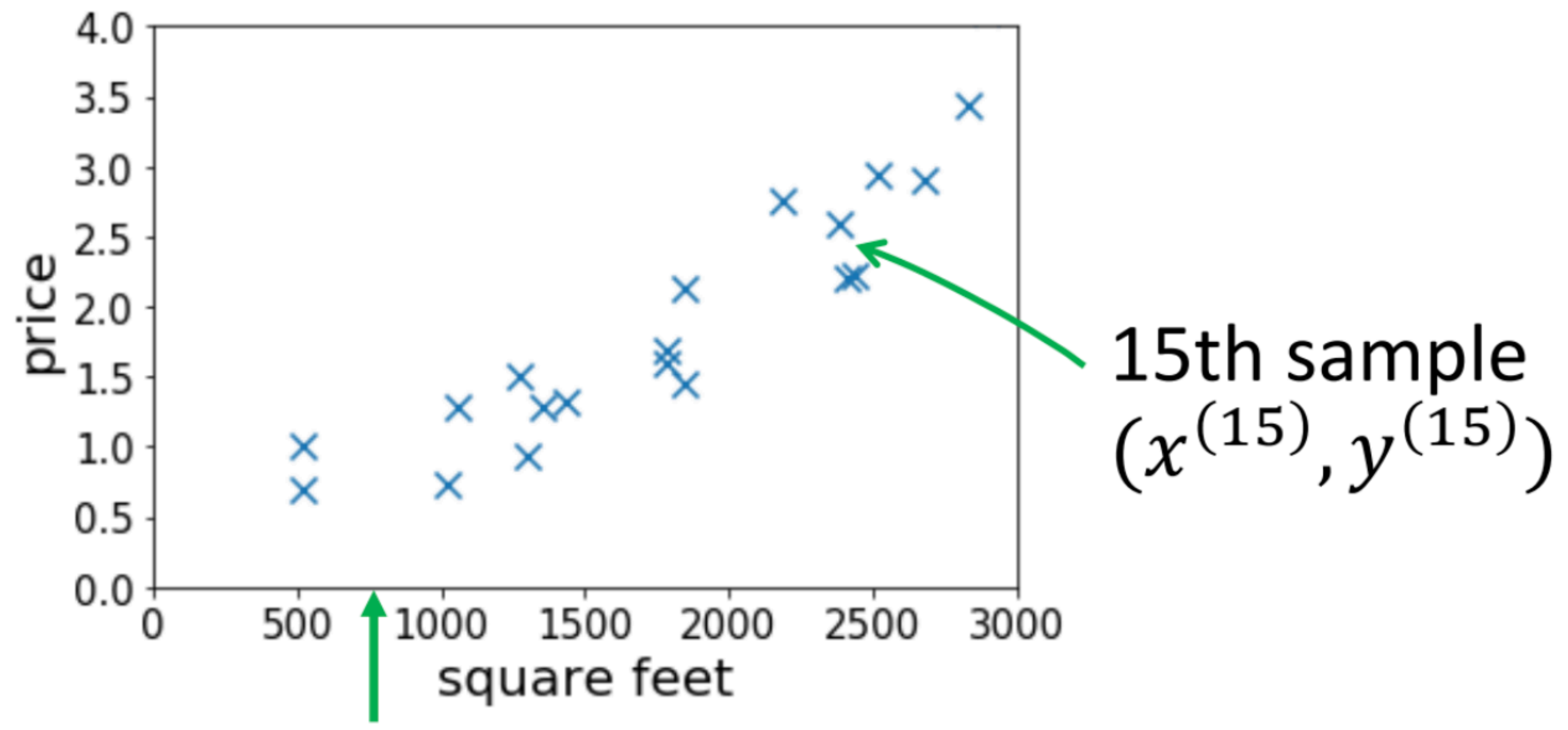
- A training set is set of pairs $\{(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)})\}$
  s.t. $x^{(i)} \in \mathcal{X}$ and $y^{(i)} \in \mathcal{Y}$ for $i = 1, \ldots, n$.

- Given a training set our goal is to produce a good prediction function h

- If $\mathcal{Y}$ is continuous, then called a regression problem
- If $\mathcal{Y}$ is discrete, then called a classification problem

Supervised Learning

- How to define "good" for a prediction function?
  - Metrics / performance



$x = 800$
$y = ?$

$$|\hat{y} - y*|$$

$\hat{y}$ is the prediction, $y*$ is the truth

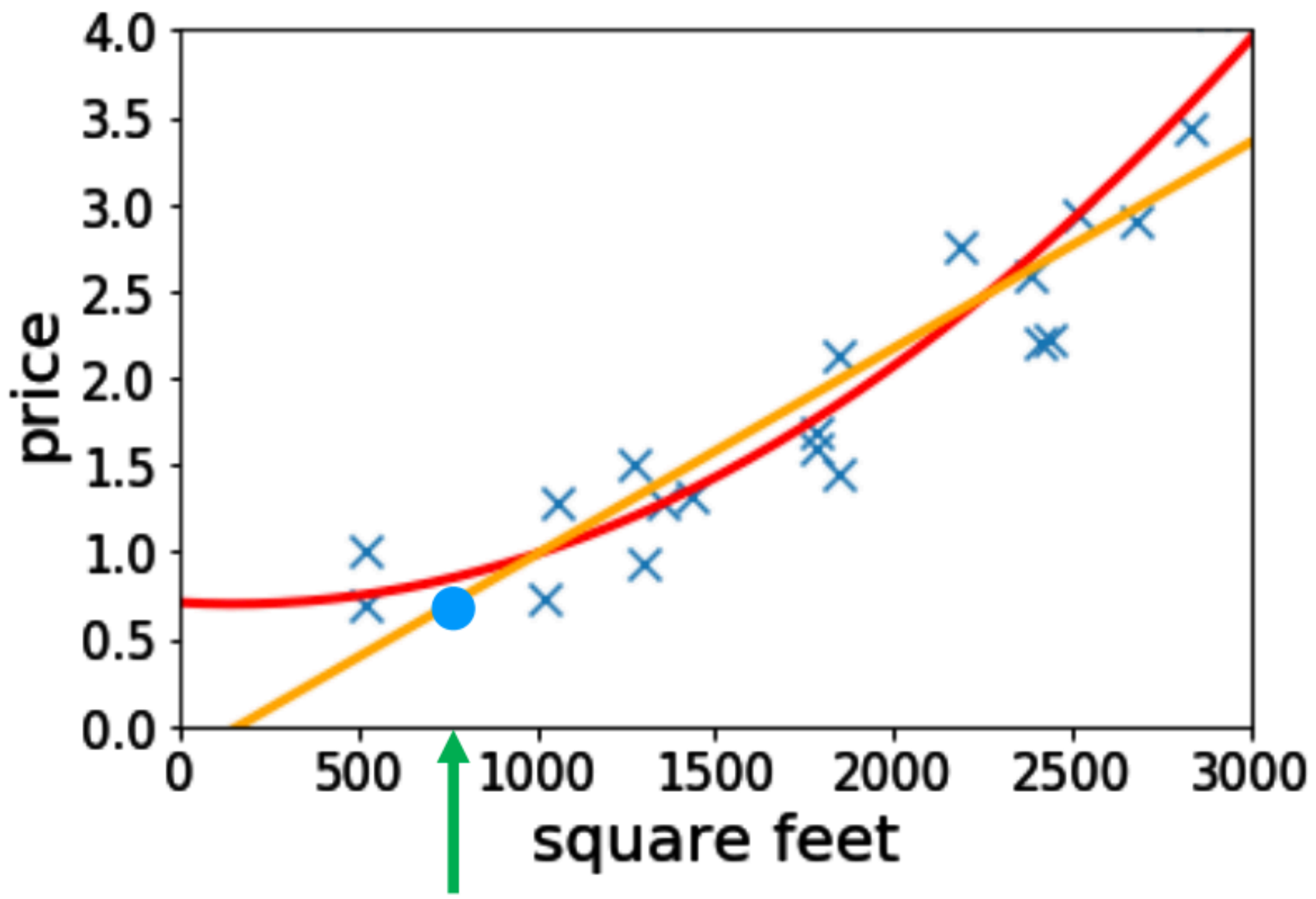
$$\mathbb{I}(\hat{y} = y*) = \begin{cases} 1, & \hat{y} = y* \\ 0 & otherwise \end{cases}$$

Supervised Learning

- How to define "good" for a prediction function?
  - Metrics / performance
  - Good on unseen data

Validation dataset is another set of pairs $\{(\hat{x}^{(1)}, \hat{y}^{(1)}), \cdots, (\hat{x}^{(m)}, \hat{y}^{(m)})\}$

Does not overlap with training dataset



Which curve to choose?

Supervised Learning

- How to define "good" for a prediction function?
  - Metrics / performance
  - Good on unseen data

Validation dataset is another set of pairs $\{(\hat{x}^{(1)}, \hat{y}^{(1)}), \cdots, (\hat{x}^{(m)}, \hat{y}^{(m)})\}$

Does not overlap with training dataset

Test dataset is another set of pairs $\{(\tilde{x}^{(1)}, \tilde{y}^{(1)}), \cdots, (\tilde{x}^{(L)}, \tilde{y}^{(L)})\}$

Does not overlap with training and validation dataset

Completely unseen before deployment

Realistic setting

Hyperparameter tuning is a form of training

Supervised Training

Train

Validation

Test

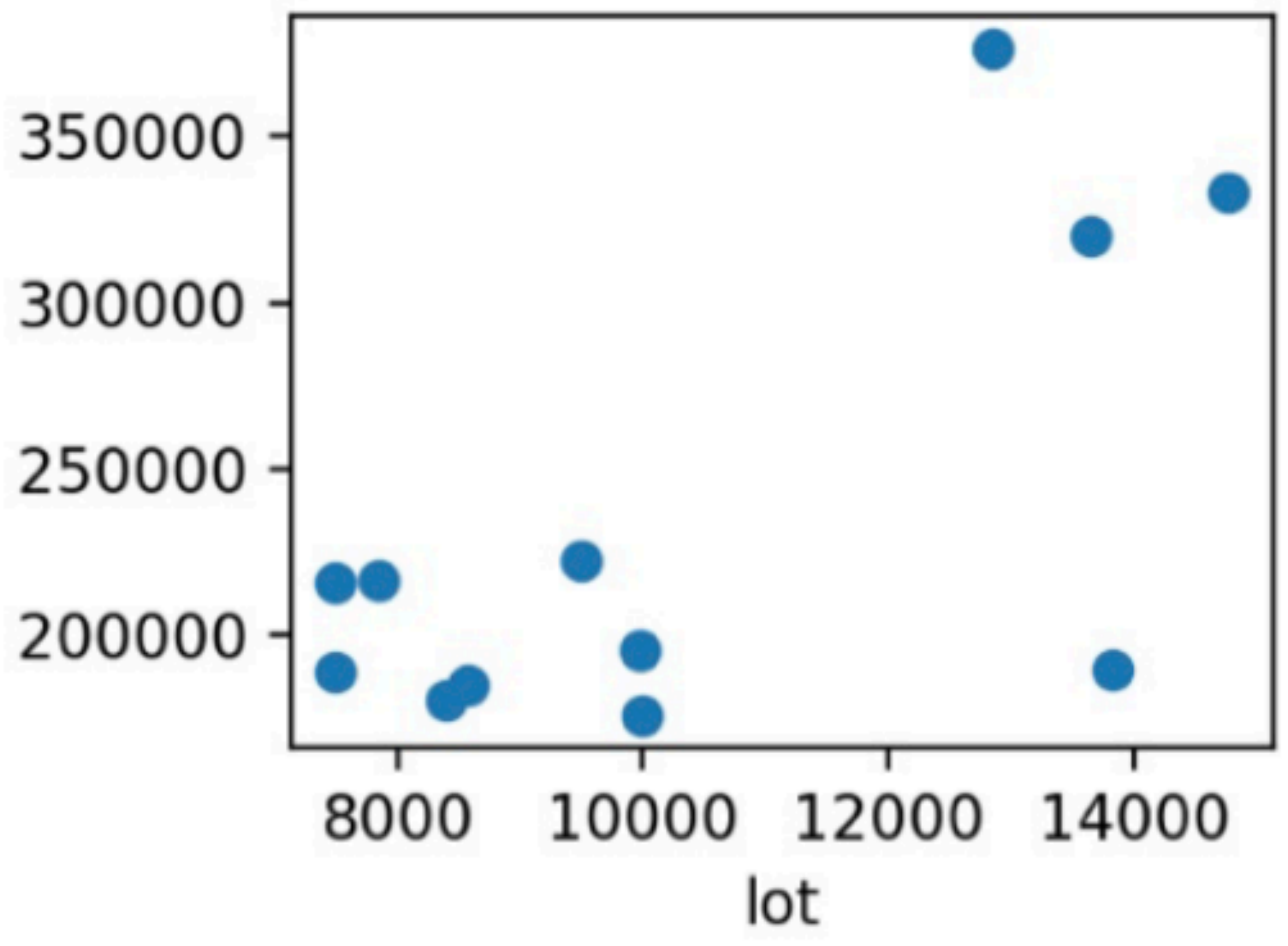
Not only for supervised learning

Example: Regression using Housing Data

Example from Stanford CS229

Example Housing Data

	SalePrice	Lot.Area
4	189900	13830
5	195500	9978
9	189000	7500
10	175900	10000
12	180400	8402
22	216000	7500
36	376162	12858
47	320000	13650
55	216500	7851
56	185088	8577



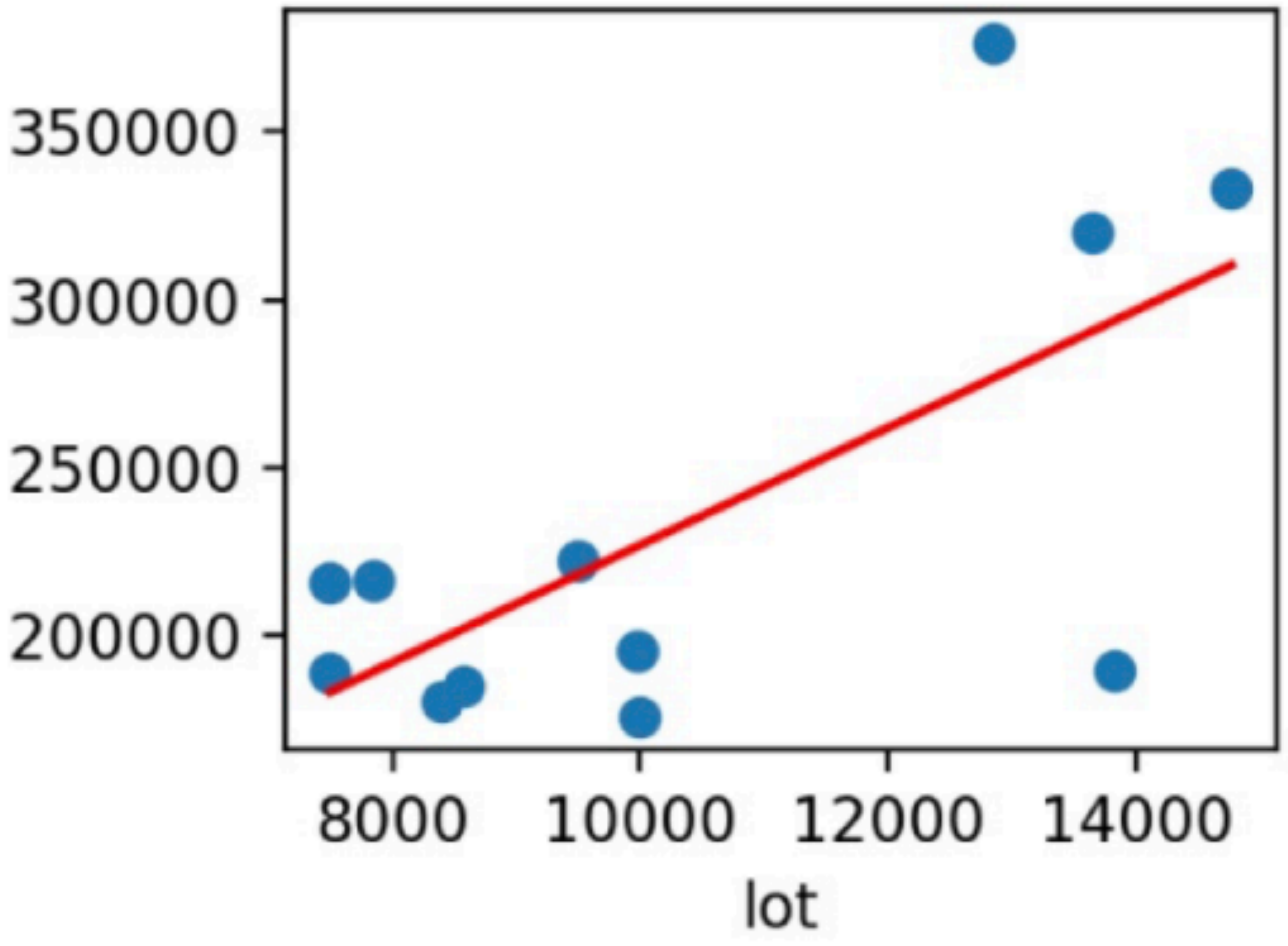
Represent h as a Linear Function

$h(x) = \theta_0 + \theta_1 x_1$ is an *affine function*

Popular choice

The function is defined by **parameters** θ_0 and θ_1, the function space is greatly reduced

Simple Line Fit



More Features

	size	bedrooms	lot size		Price
$x^{(1)}$	2104	4	45k	$y^{(1)}$	400
$x^{(2)}$	2500	3	30k	$y^{(2)}$	900

What's a prediction here?

$$h(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3.$$

With the convention that $x_0 = 1$ we can write:

$$h(x) = \sum_{j=0}^{3} \theta_j x_j$$

Vector Notations

	size	bedrooms	lot size
$x^{(1)}$	2104	4	45k
$x^{(2)}$	2500	3	30k

	Price
$y^{(1)}$	400
$y^{(2)}$	900

We write the vectors as (important notation)

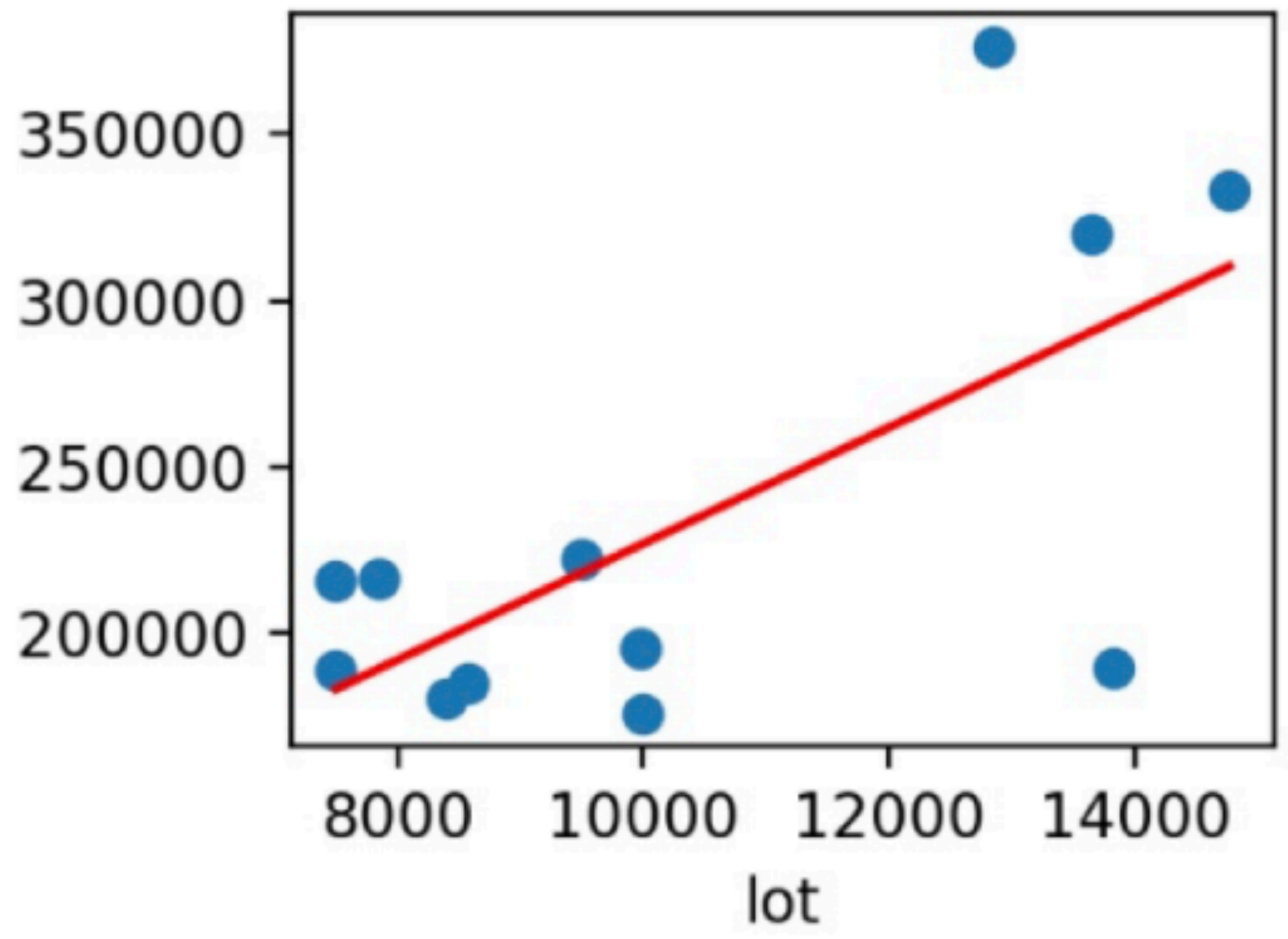
$$\theta = \begin{pmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \theta_3 \end{pmatrix} \text{ and } x^{(1)} = \begin{pmatrix} x_0^{(1)} \\ x_1^{(1)} \\ x_2^{(1)} \\ x_3^{(1)} \end{pmatrix} = \begin{pmatrix} 1 \\ 2104 \\ 4 \\ 45 \end{pmatrix} \text{ and } y^{(1)} = 400$$

We call θ **parameters**, $x^{(i)}$ is the input or the **features**, and the output or **target** is $y^{(i)}$. To be clear,

(x, y) is a training example and $(x^{(i)}, y^{(i)})$ is the i^{th} example.

We have n examples. There are d features. $x^{(i)}$ and θ are d+1 dimensional (since $x_0 = 1$)

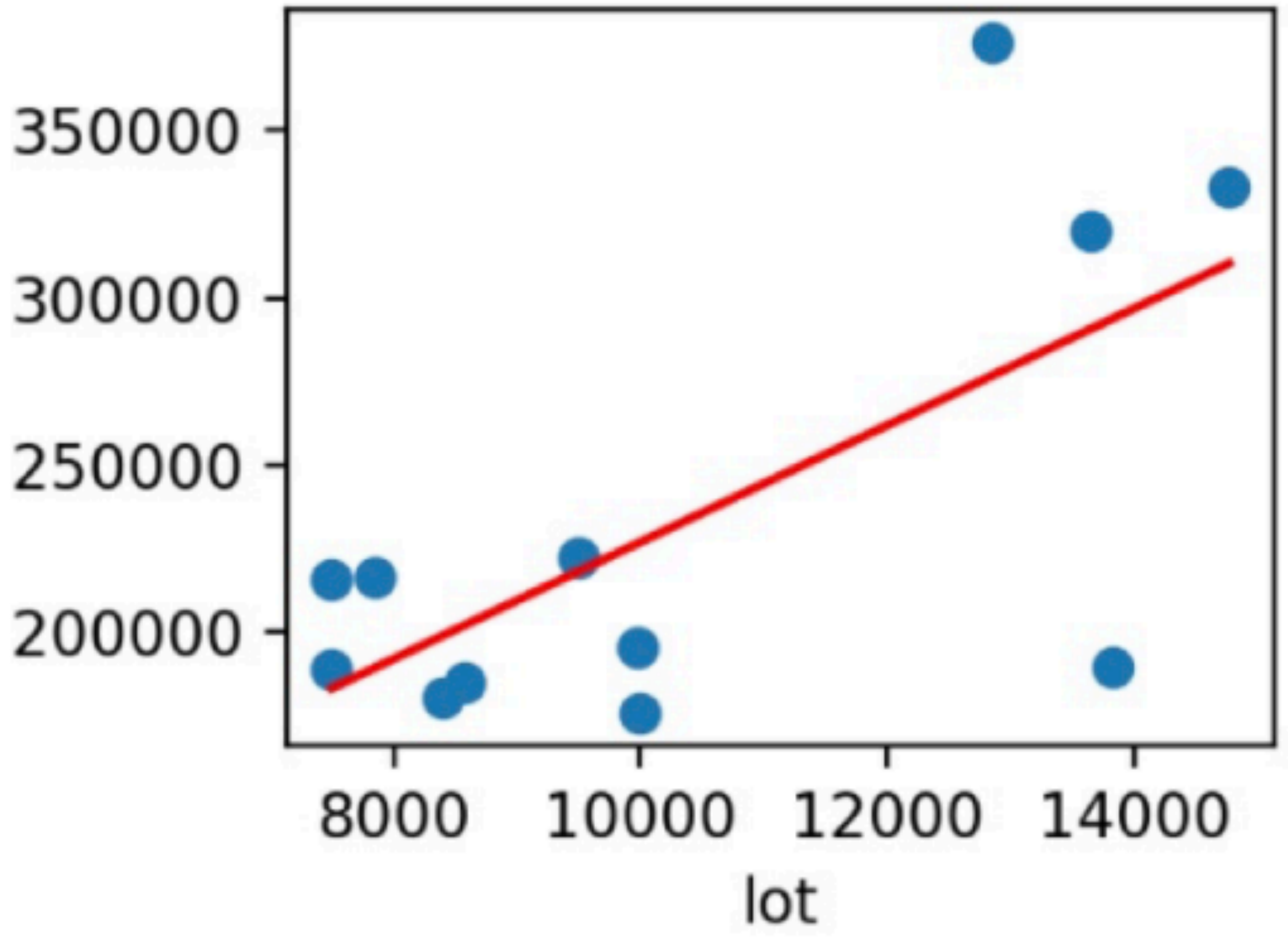
Vector Notation of Prediction



$$h_\theta(x) = \sum_{j=0}^{d} \theta_j x_j = x^T \theta$$

We want to choose θ so that $h_\theta(x) \approx y$

Loss Function

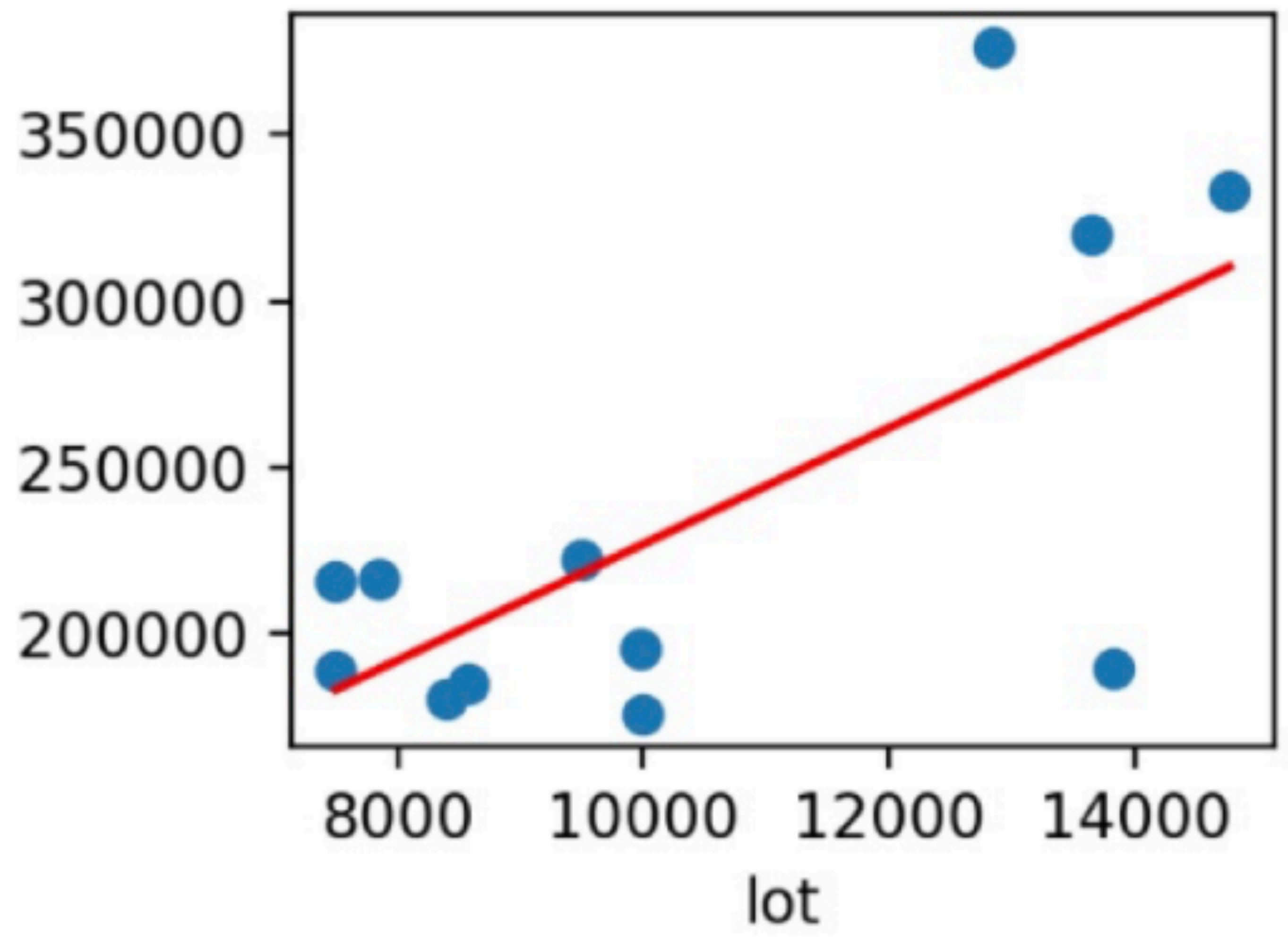


$$h_\theta(x) = \sum_{j=0}^{d} \theta_j x_j = x^T\theta$$

We want to choose θ so that $h_\theta(x) \approx y$

How to quantify the deviation of $h_\theta(x)$ from y

Least Squares



$$h_\theta(x) = \sum_{j=0}^{d} \theta_j x_j = x^T\theta$$

$$J(\theta) = \frac{1}{2}\sum_{i=1}^{n}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$

Choose

$$\theta = \operatorname*{argmin}_\theta J(\theta).$$

Solving Least Square Problem

Direct Minimization

$$h_\theta(x) = \sum_{j=0}^{d} \theta_j x_j = x^T \theta \qquad\qquad J(\theta) = \frac{1}{2} \sum_{i=1}^{n} \left(h_\theta(x^{(i)}) - y^{(i)} \right)^2$$

Choose

$$\theta = \underset{\theta}{\operatorname{argmin}}\, J(\theta).$$

Solving Least Square Problem

$$\begin{aligned}
\nabla_\theta J(\theta) &= \nabla_\theta \frac{1}{2}(X\theta - \vec{y})^T(X\theta - \vec{y}) \\
&= \frac{1}{2}\nabla_\theta \left((X\theta)^T X\theta - (X\theta)^T\vec{y} - \vec{y}^T(X\theta) + \vec{y}^T\vec{y}\right) \\
&= \frac{1}{2}\nabla_\theta \left(\theta^T(X^TX)\theta - \vec{y}^T(X\theta) - \vec{y}^T(X\theta)\right) \\
&= \frac{1}{2}\nabla_\theta \left(\theta^T(X^TX)\theta - 2(X^T\vec{y})^T\theta\right) \\
&= \frac{1}{2}\left(2X^TX\theta - 2X^T\vec{y}\right) \\
&= X^TX\theta - X^T\vec{y}
\end{aligned}$$

Normal equations $X^TX\theta = X^T\vec{y}$ $\qquad \theta = (X^TX)^{-1}X^T\vec{y}.$

When is X^TX invertible? What if it is not invertible?

Thank You!

Q & A