Recap

- Univariate distributions
- Delete outliers, StandardScaler
- Retain outliers, RobustScaler
- Or use distribution transformation on features to make outliers into inliers
  - Log Transformer
  - FunctionTransformers
  - PowerTransformers – Box Cox, Yeo Johnson

3rd method - Analyzing outliers for detection

- Focus on outliers and not regular data
- No deletion or scaling
- Exclusively analyze data > 2.5 standard deviation or later by applying specific mathematical approaches
- Interesting & relevant topic in industry
- We will only be briefly looking at this ☹

Cons of our approach so far (from outlier perspective)

- Can we just look at the standard deviations or IQR of each feature individually?
- Each data point is multivariate in reality
- Analysis also needs to be holistic
- Enter multivariate probability density functions

Why look at probability at all in ML course?

- Needed for generative ML (soon in Sem1)
  - Maximum Likelihood Estimation (MLE/MAP)
- Needed for information theory refresher
  - Used in Decision Trees & ensembles
  - Used in Feature Selection
- Generative AI
- Probabilistic Deep Learning (Bayesian Neural Networks)
- Using this opportunity to introduce multivariate distributions

EfficientNet trained on ImageNet images

Prediction: Typewriter
Certainty: 85%

Prediction: Stonewall
Certainty: 87%

ImageNet is a 1000 class dataset !!

Multivariate distributions

Expected value

- Weighted average to probability based formulation

$$\mathbb{E}[X] = \sum_x x p(x)$$

$$\mathbb{E}[f(X)] = \sum_x f(x) p(x)$$

$$\mathbb{E}[\alpha X + \beta Y] = \alpha \mathbb{E}[X] + \beta \mathbb{E}[Y]$$

- Why Expectation?
  - Hint: Linear operator

Standard deviation method (contd.)

- Standard deviation is the typical deviation of feature value from mean

Put mu for E[X] and then expand to see for yourself

$$\sigma = \sqrt{\frac{1}{n}\Sigma_{i=1}^{n}(x_i - \mu)^2} \qquad = \frac{\|x - \mu\mathbf{1}\|}{\sqrt{n}}$$

$$\sigma^2 = \mathbb{E}[(X - \mathbb{E}[X])^2] \qquad = \mathbb{E}[X^2] + \mathbb{E}[\mathbb{E}[X]]^2 - 2\mathbb{E}[X\mathbb{E}[X]]$$

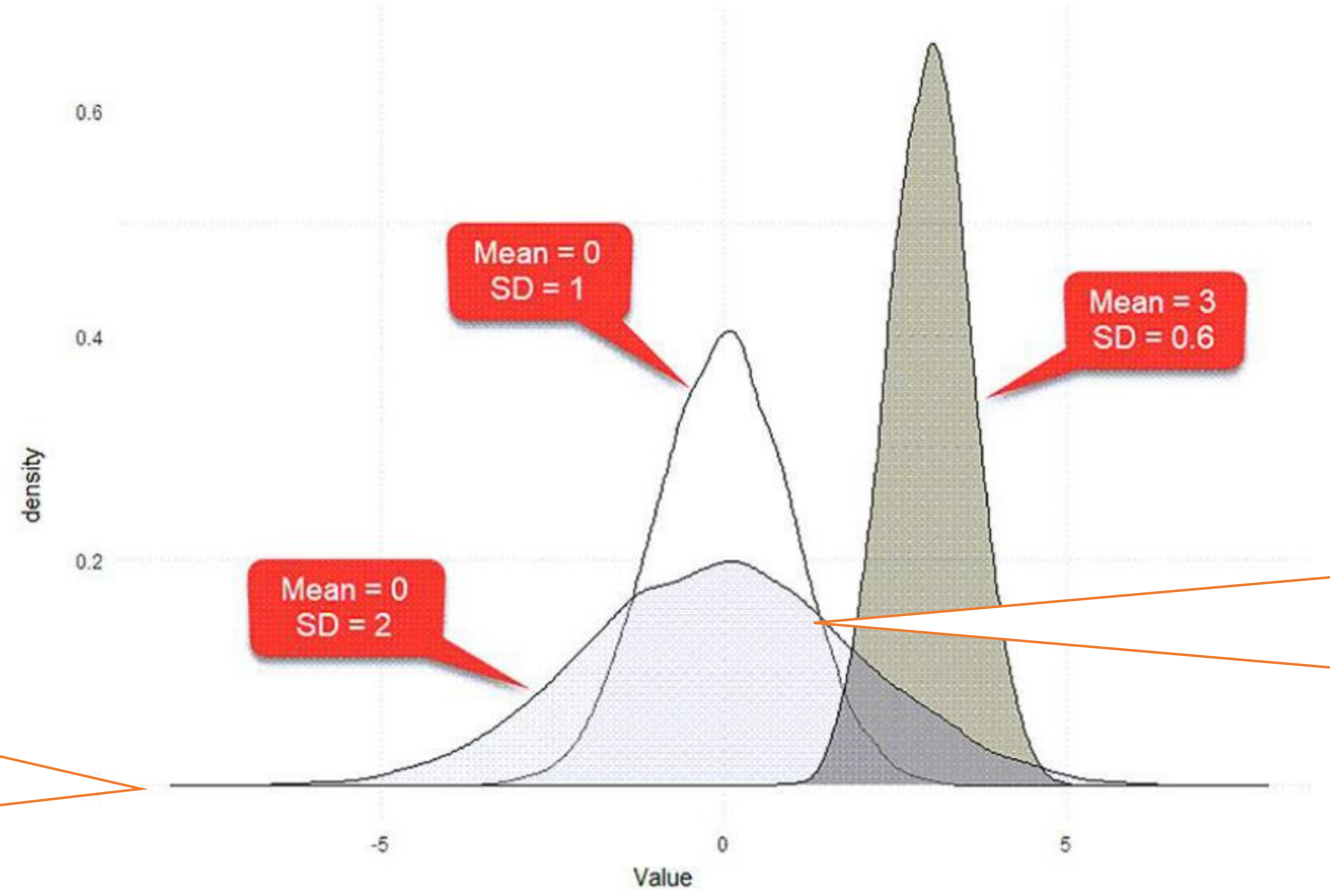
$$= \mathbb{E}[X^2] + \mathbb{E}[X]^2 - 2\mathbb{E}[X]^2 \qquad = \mathbb{E}[X^2] - \mathbb{E}[X]^2$$

Note for M.E students. This is the Linear Algebra equivalent

$$std(x)^2 = rms(x)^2 - avg(x)^2$$

Univariate distribution

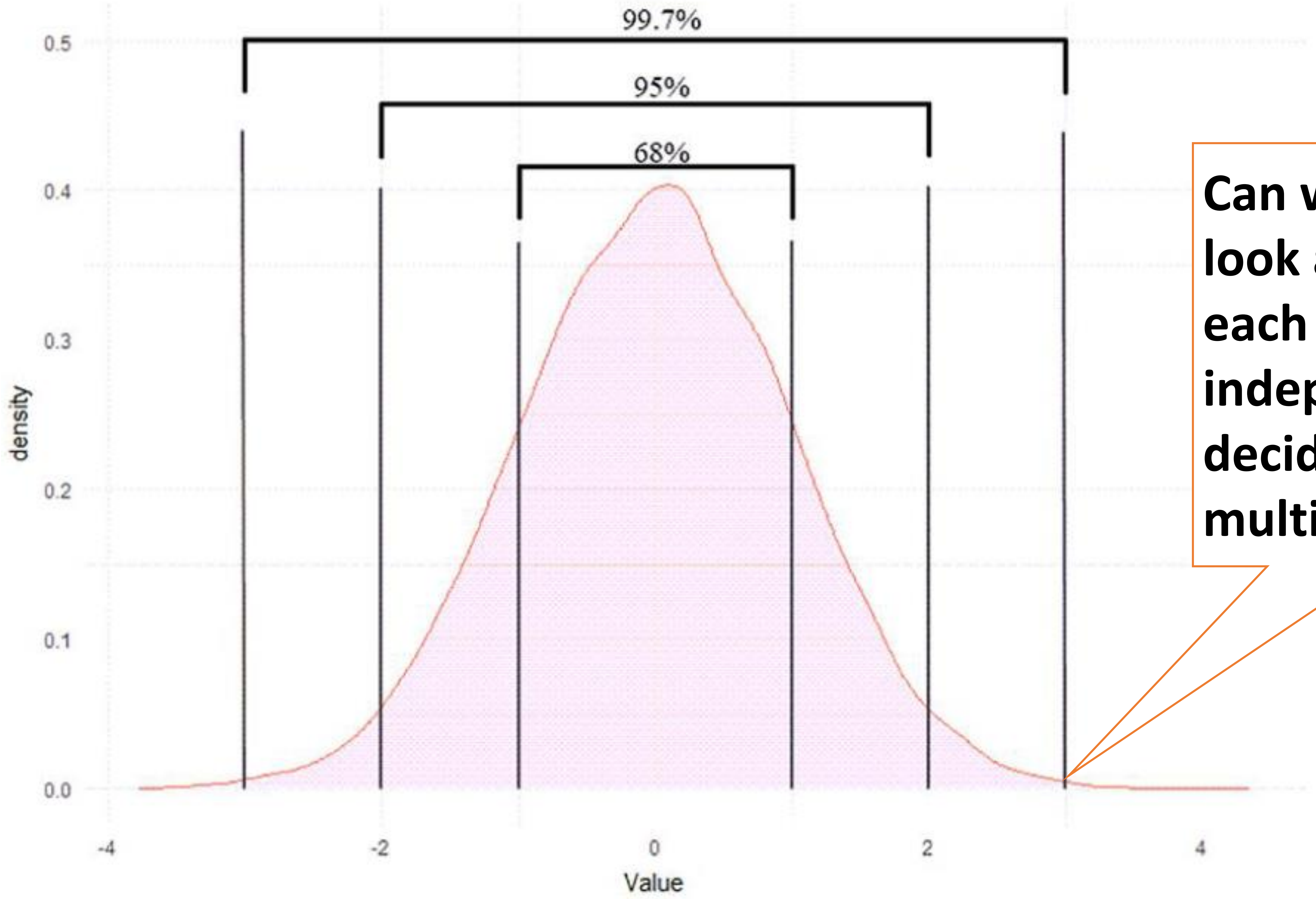
- A univariate Gaussian $X \sim \mathcal{N}(\mu, \sigma^2)$ $\frac{1}{\sqrt{2\pi\sigma^2}} e^{\frac{-1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$



Random variable X

Why does height decrease as the distribution becomes wide?

Empirical Formula for Gaussian Distribution

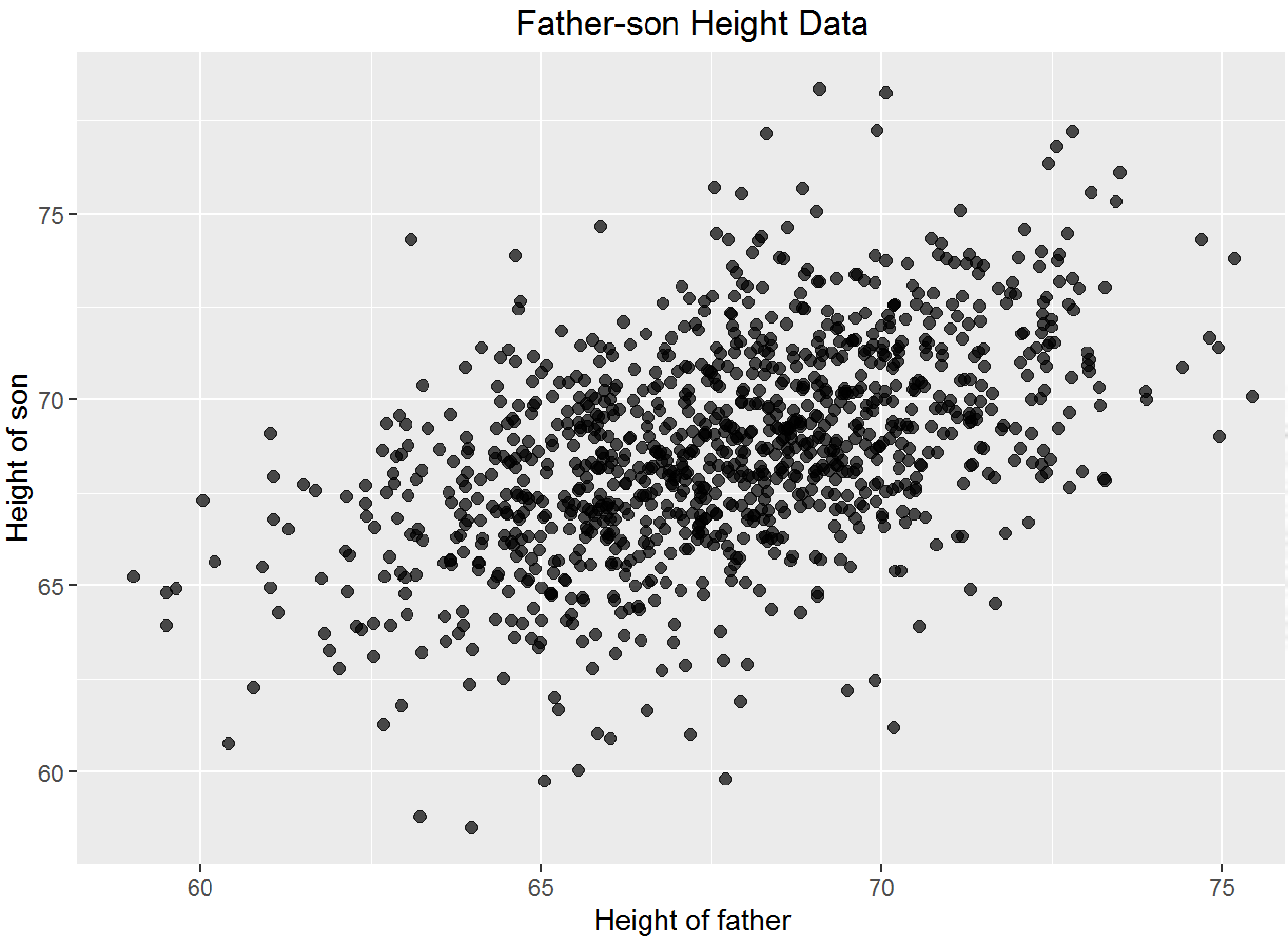


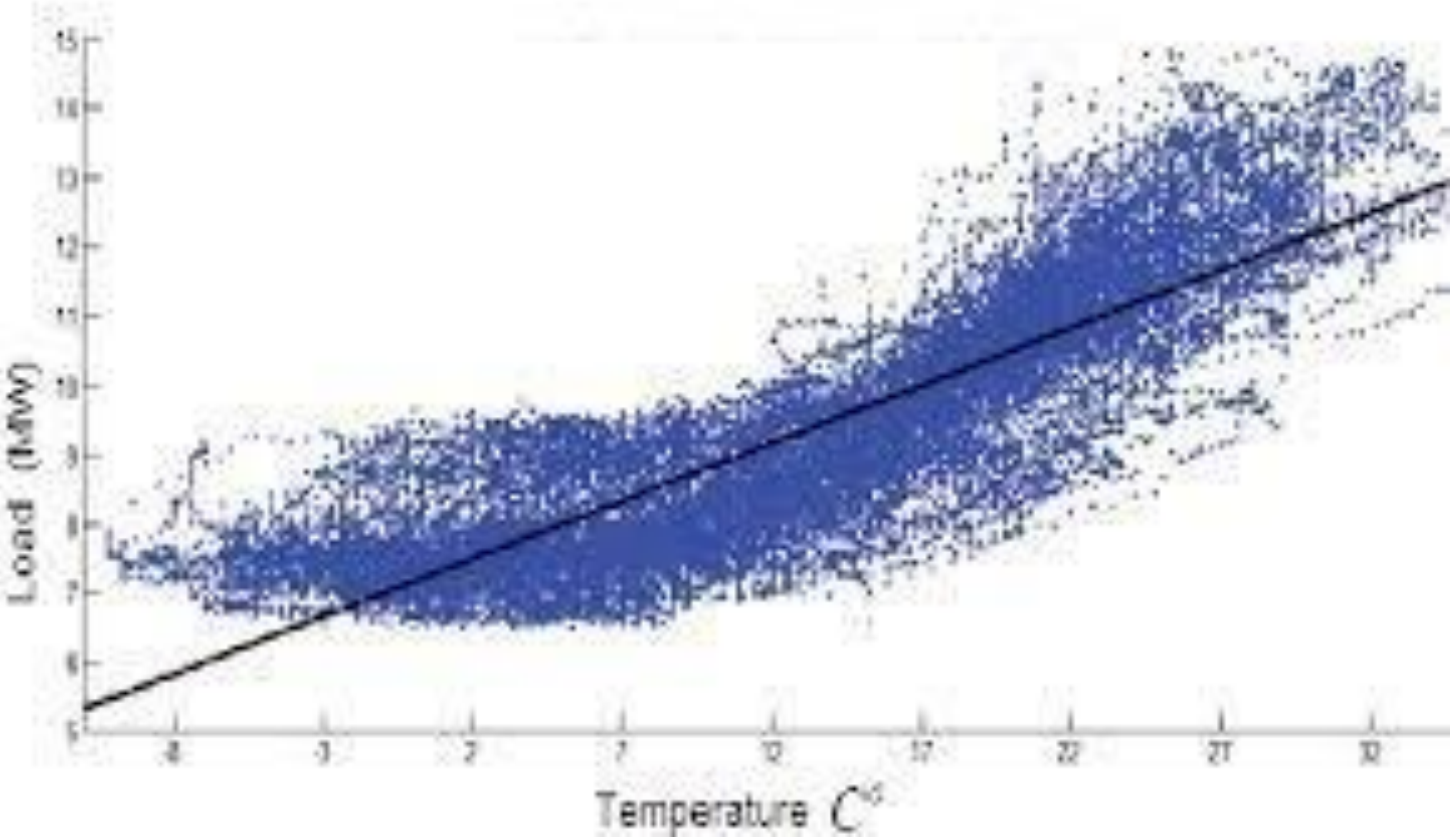
Can we REALLY look at 3 SD for each feature independently to decide and delete multivariate data?

Correlation

Correlation

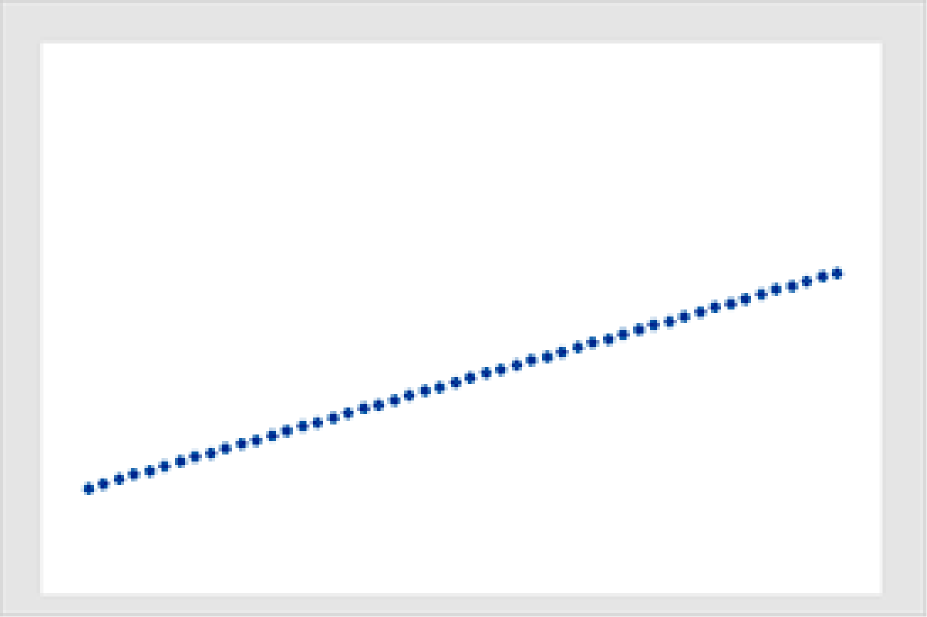
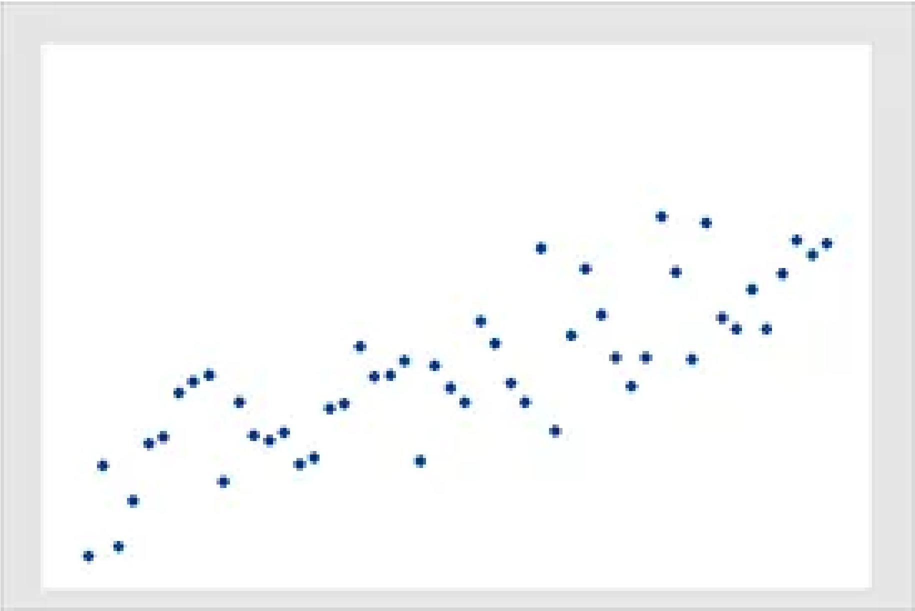
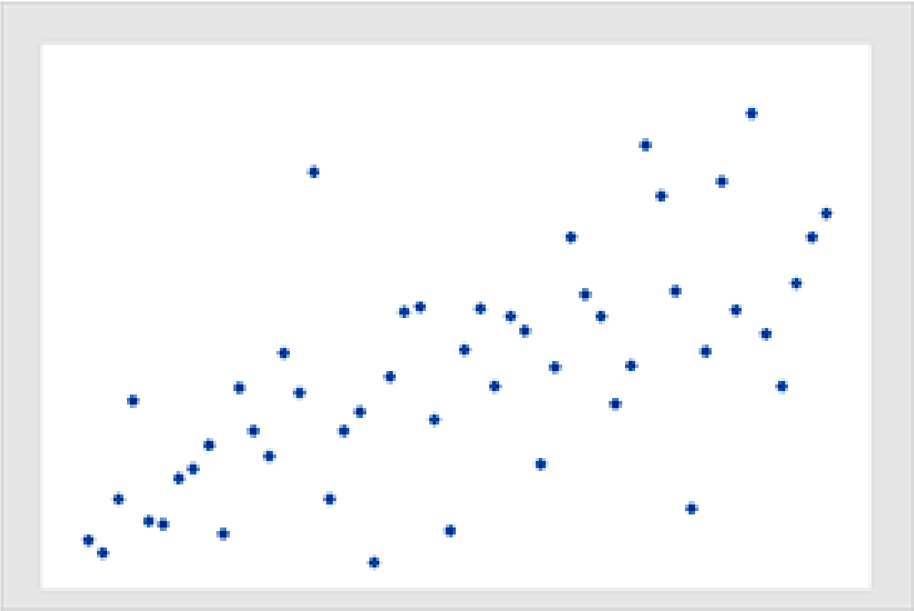
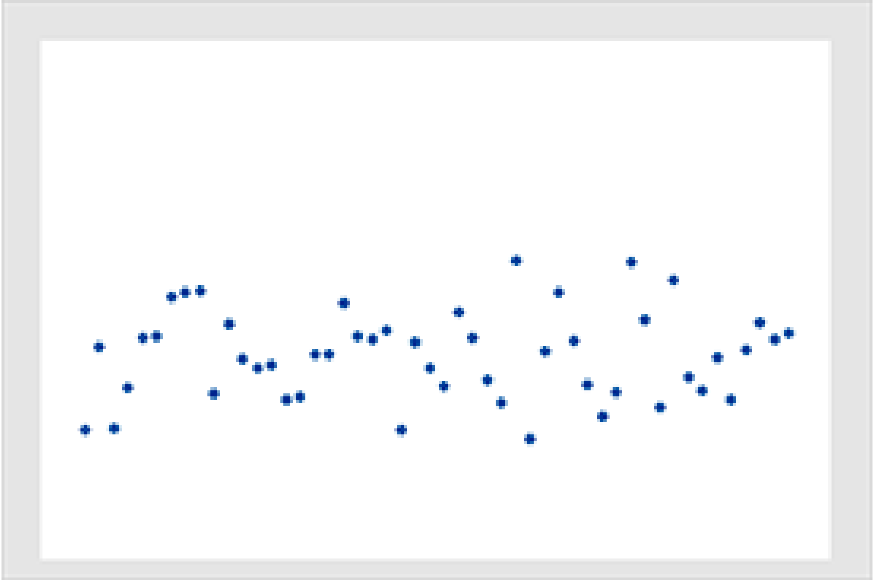
- Father-son heights
- Temperature-Electric bill



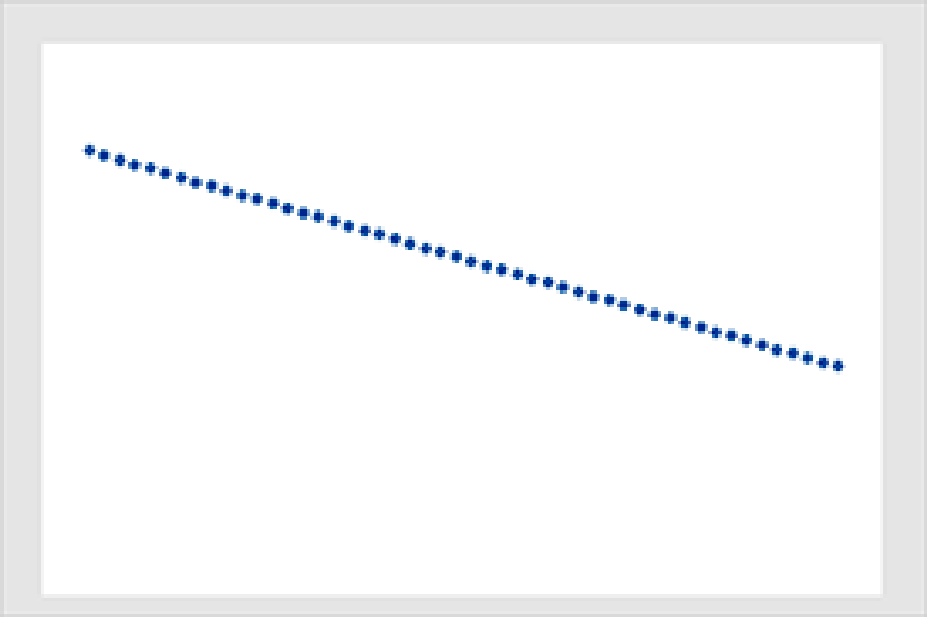


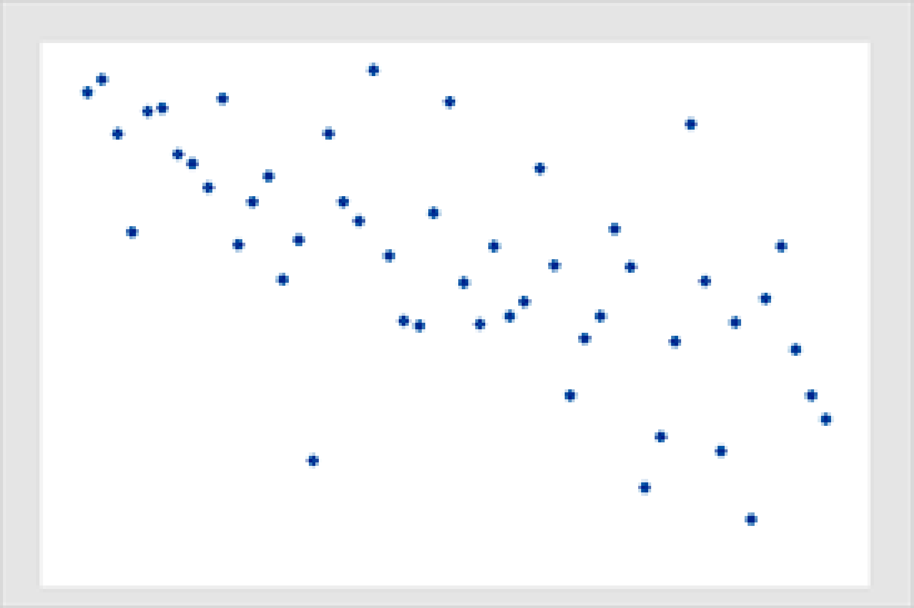
Correlation strength & coefficients

- Very Strong Strong Moderate None

- 1 0.8 0.6 0
- -1 -0.8 -0.6





Correlation coefficient

- Covariance and Correlation are bivariate

$$Cov(x,y) = \frac{\Sigma_{i=1}^{n}(x-\bar{x})(y-\bar{y})}{n} \quad = \mathbb{E}[(X-\mathbb{E}[X])(Y-\mathbb{E}[Y])]$$

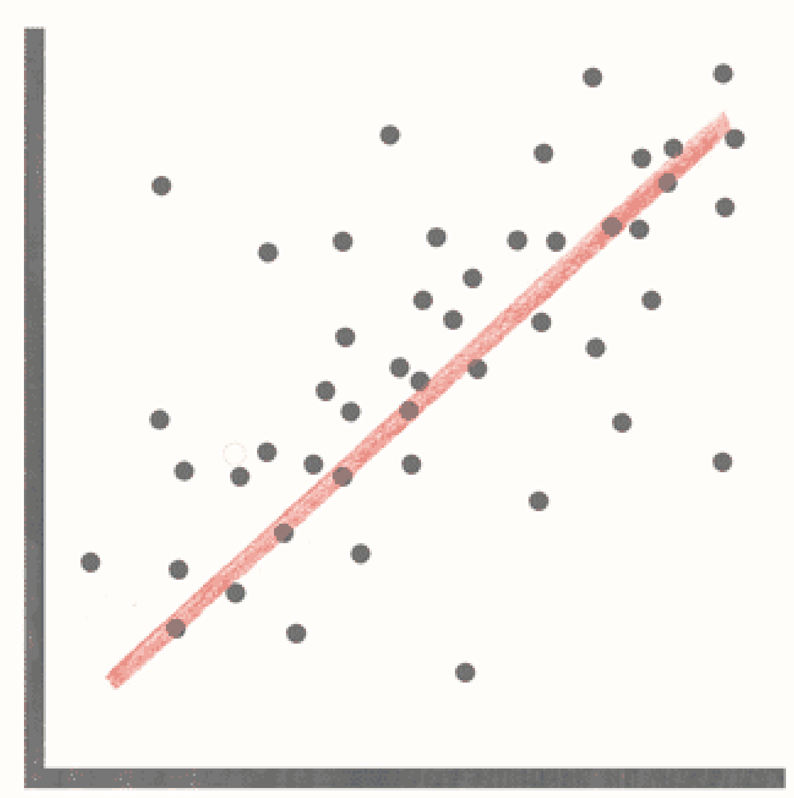
$$= \mathbb{E}[XY] - \mathbb{E}[X])\mathbb{E}[Y]$$

Cov(x,x) = Var(x)

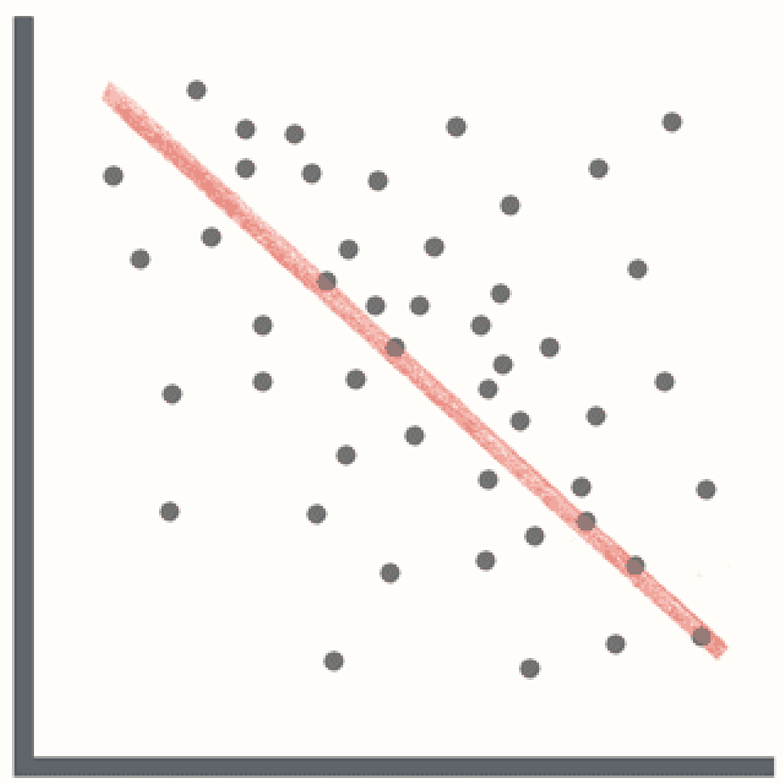
$$\rho = Correl(x,y) = \frac{Cov(x,y)}{\sigma_x \sigma_y}$$

$$\rho = \frac{1}{n}\Sigma_{i=1}^{n}\left(\frac{x_i-\bar{x}}{\sigma_x}\right)\left(\frac{y_i-\bar{y}}{\sigma_y}\right)$$

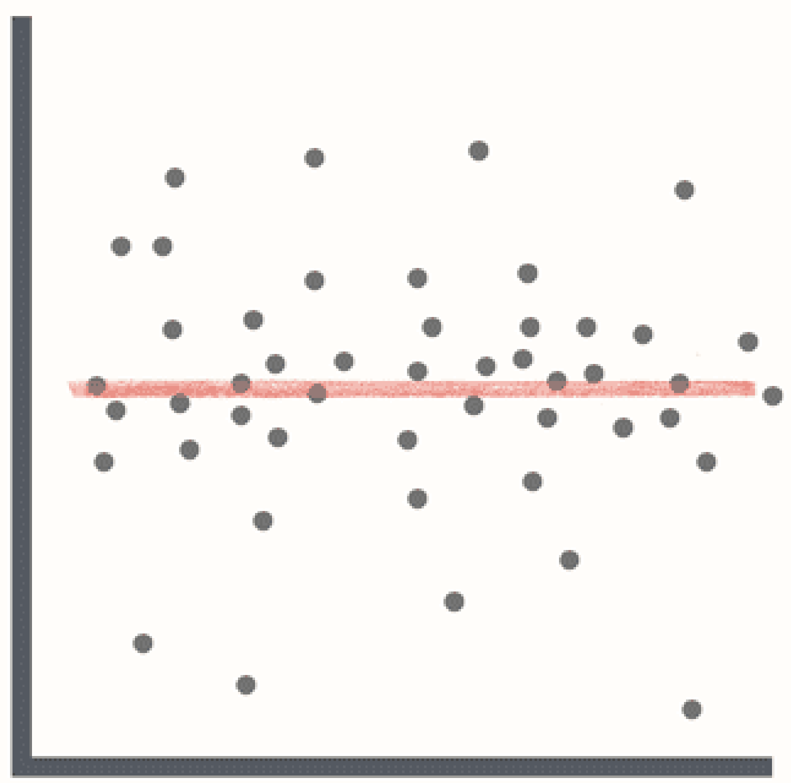
Intuition behind mean centering



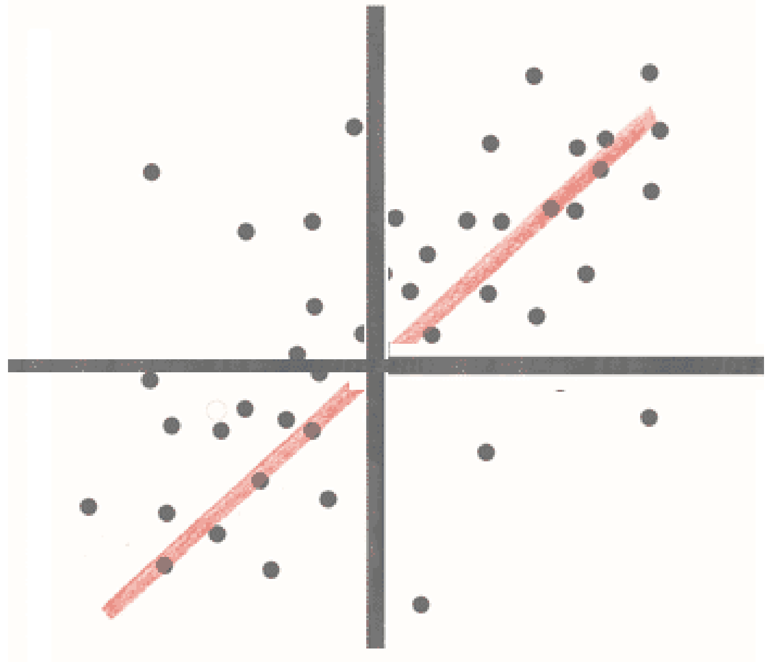
Positive Correlation



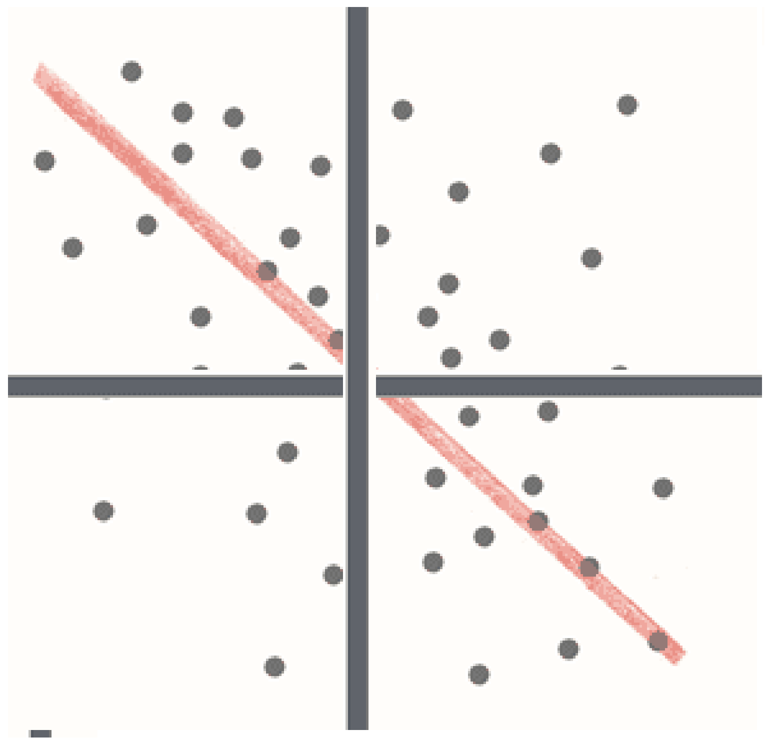
Negative Correlation



No Correlation



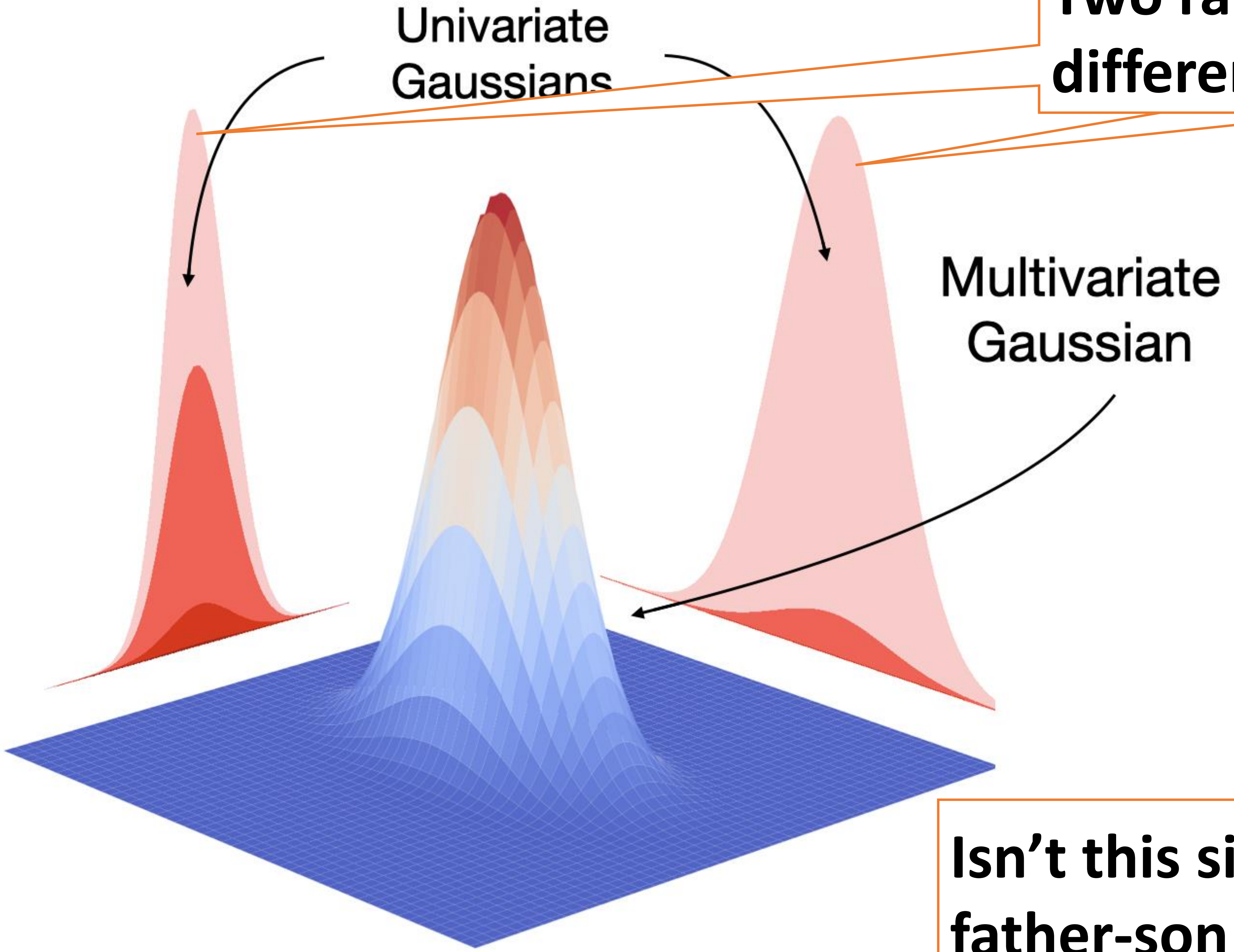
Positive Correlation



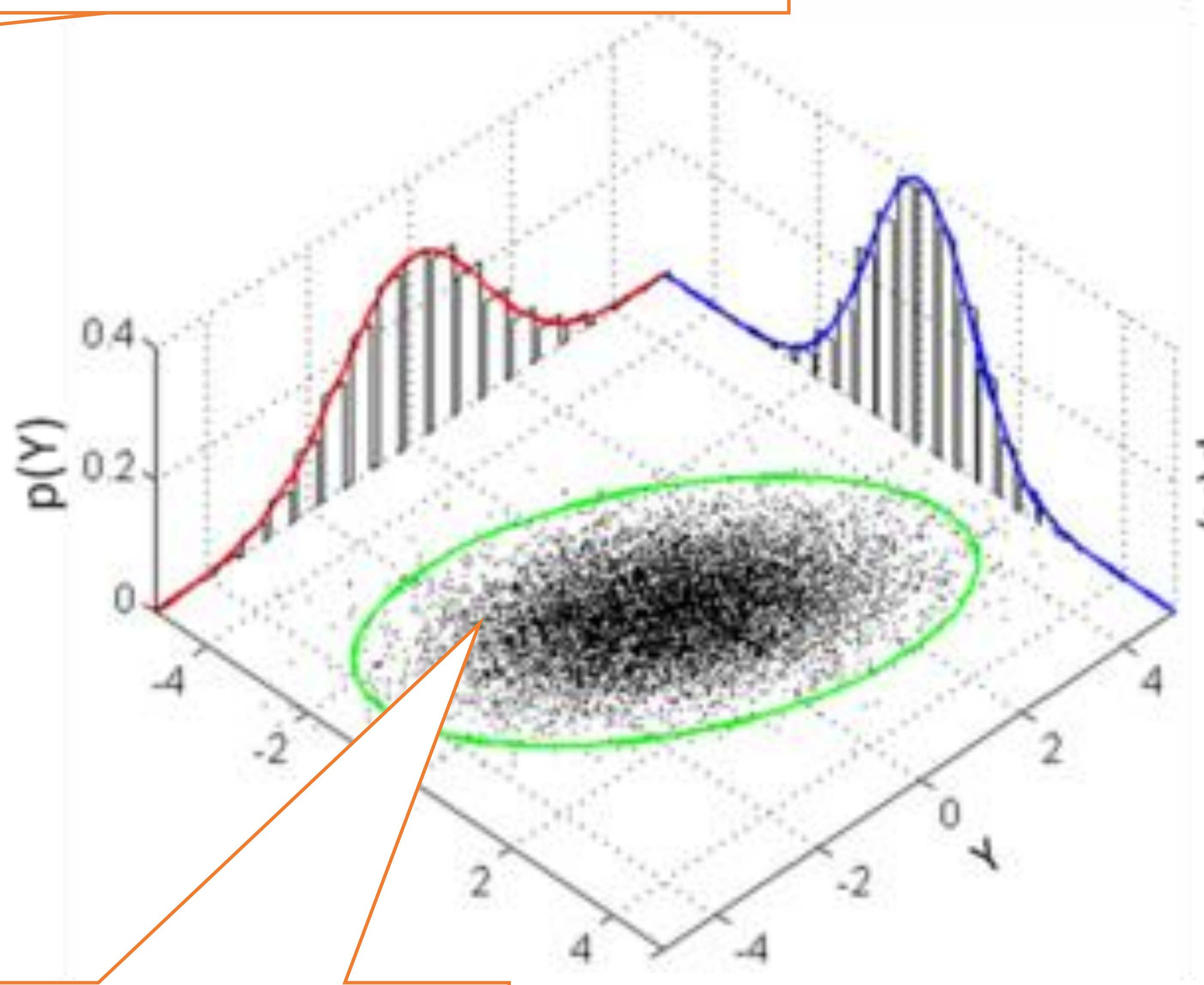
Correlation is not causation

Bivariate Gaussian

Multivariate Gaussian



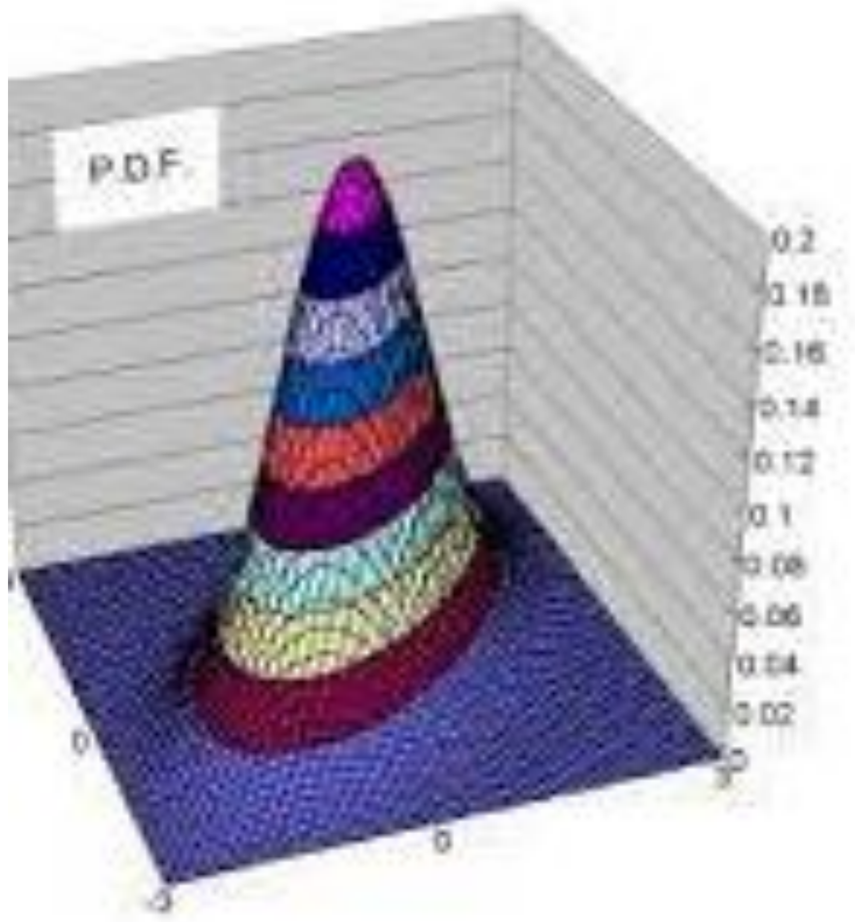
Two random variable with different mean and SD



Isn't this similar to father-son height covariance plot?

Interpreting contour plots

- Multivariate Gaussian
  - https://www.geogebra.org/m/pO4JcWPz
- Contour plots (Isocontours)
  - Slicing through the function surface for a fixed z



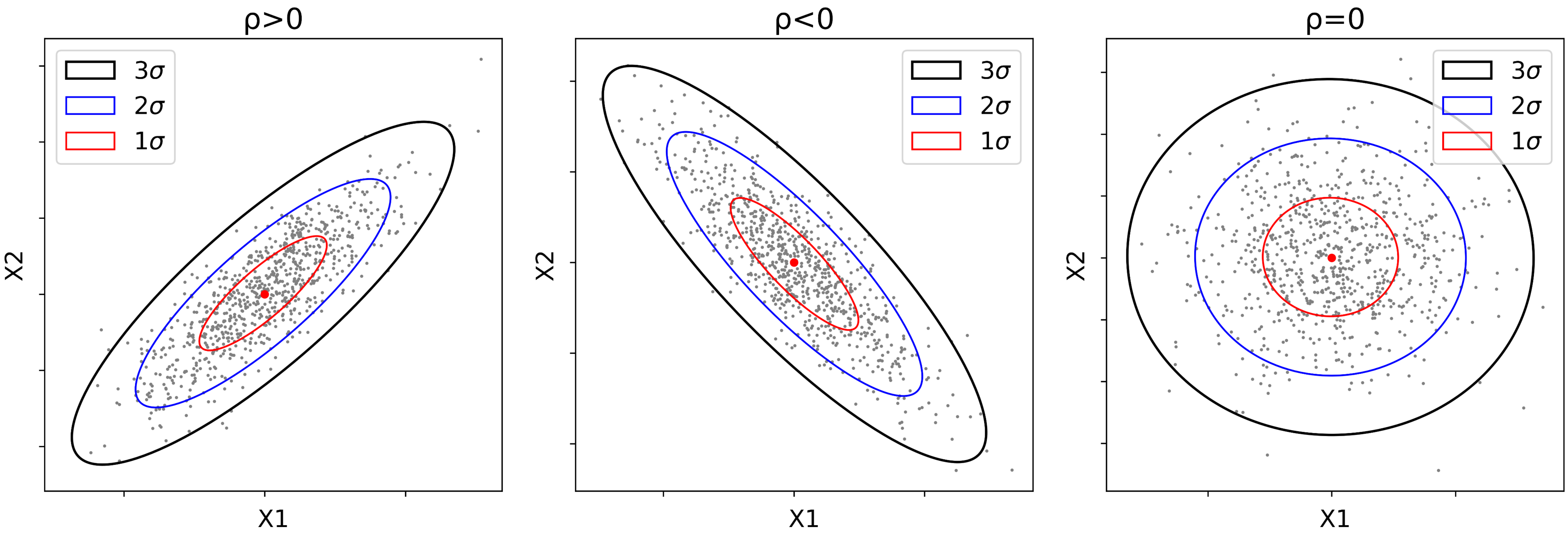
Multivariate Gaussian formula intuition

- We saw bivariate distribution as having two random variables with different mean and SD

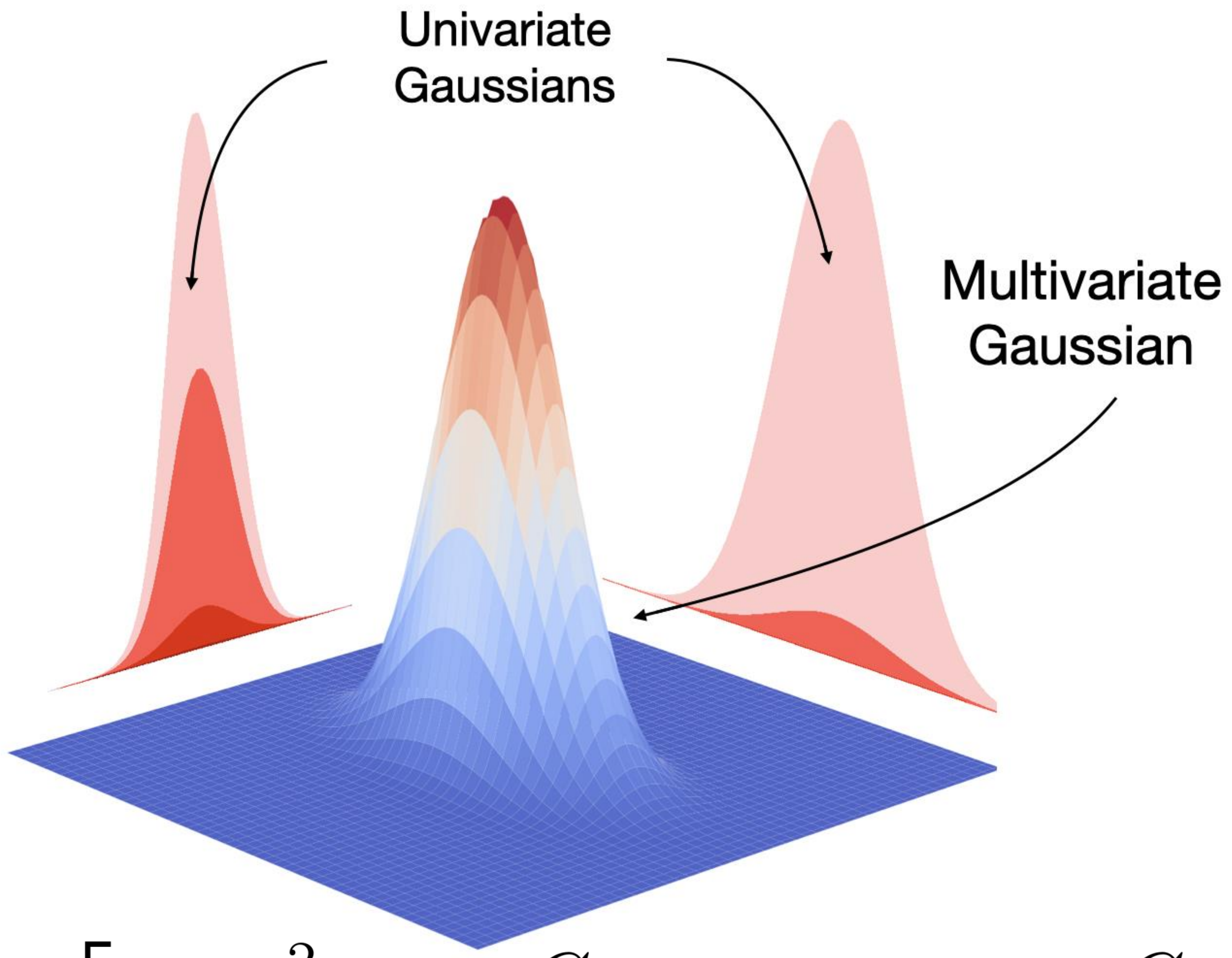
$$X = \begin{bmatrix} X_1 \\ X_2 \end{bmatrix}$$

Distribution of random vector X by also taking into account the interaction between RV

- What do we mean by interaction?
  - Recall father son heights
  - Student absent days versus grade
  - Google stock prices versus ice cream num sold



- Multivariate Gaussian formula should take into account the correlation/covariance based interaction



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

Multivariate Gaussian formula should have mean & SD for both random variables in vector

$$\mu = \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix} \quad \sigma = \begin{bmatrix} \sigma_1 \\ \sigma_2 \end{bmatrix}$$

$$\Sigma = \begin{bmatrix} \sigma_1^2 & Cov_{12} & \dots & Cov_{1n} \\ Cov_{21} & \sigma_2^2 & \dots & Cov_{2n} \\ .. & .. & .. & .. \\ Cov_{(n-1)1} & .. & \sigma_{n-1}^2 & Cov_{(n-1)n} \\ Cov_{n1} & Cov_{n2} & .. & \sigma_n^2 \end{bmatrix}$$

$$Cov(x,y) = \frac{\Sigma_{i=1}^{n}(x-\bar{x})(y-\bar{y})}{n}$$

Why have a matrix when scalar cov are duplicated?

Univariate

Normalization constant

$$X \sim \mathcal{N}(\mu, \sigma^2)$$

$$\frac{1}{\sqrt{2\pi\sigma^2}} e^{\frac{-1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$$

Bell shape bcoz of this

$$\mathbf{X} = \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} \qquad \mu = \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix} \qquad \sigma = \begin{bmatrix} \sigma_1 \\ \sigma_2 \end{bmatrix} \qquad \sum$$

Cov matrix already holds all SD

Multivariate

$$\mathbf{X} \sim \mathcal{N}(\mu, \Sigma)$$

Multivariate

$$\mathbf{X} \sim \mathcal{N}(\mu, \Sigma)$$

$$\boxed{\frac{1}{\sqrt{\sigma^2 2\pi}} e^{\frac{-1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}}$$

X is a vector. Mu is a vector. Can you square a vector?

$$e^{\frac{-1}{2}\left(\frac{\mathbf{X}-\mu}{\sigma}\right)^2}$$

Quadratic form giving scalar

$$x^T x = \|x\|^2$$

$$e^{\frac{-1}{2}(\mathbf{X}-\mu)^T \ldots (\mathbf{X}-\mu)}$$

How to account for spread of two random variables & their interaction (joint spread)?

Account for 3 scalars capturing the spread

Spread goes to denominator

$$e^{\frac{-1}{2}(\mathbf{X}-\mu)^T \Sigma (\mathbf{X}-\mu)}$$

$$e^{\frac{-1}{2}(\mathbf{X}-\mu)^T \Sigma^{-1} (\mathbf{X}-\mu)}$$

Normalization constant

$$\frac{1}{\sqrt{det(\Sigma)(2\pi)^D}} e^{\frac{-1}{2}(\mathbf{X}-\mu)^T \Sigma^{-1} (\mathbf{X}-\mu)}$$

Uni v/s multivariate similarities

Univariate

$$\frac{1}{\sqrt{\sigma^2 2\pi}} e^{\frac{-1}{2}(\frac{x-\mu}{\sigma})^2}$$

$$\sigma > 0$$

Multivariate

$$\frac{1}{\sqrt{det(\Sigma)(2\pi)^D}} e^{\frac{-1}{2}(\mathbf{X}-\mu)^T \Sigma^{-1} (\mathbf{X}-\mu)}$$

$$\sum > 0 \qquad \Sigma = \begin{bmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{21} & \sigma_2^2 \end{bmatrix}$$

- Covariance matrix is symmetric positive definite
- Symmetric is easy to see
- Positive definite means Eigen values > 0

Uni v/s multivariate similarities(contd.)

Univariate

$$\frac{1}{\sqrt{\sigma^2 2\pi}} e^{\frac{-1}{2}(\frac{x-\mu}{\sigma})^2}$$

$$z = \frac{x-\mu}{\sigma}$$

Multivariate

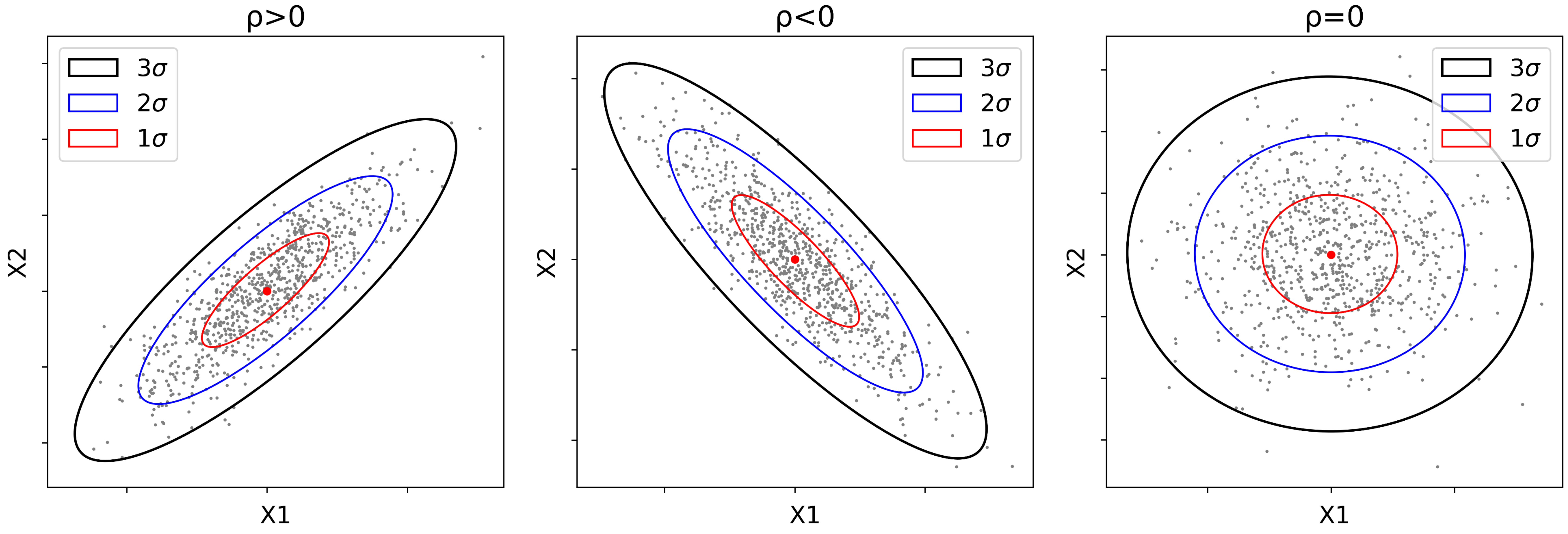
$$\frac{1}{\sqrt{det(\Sigma)(2\pi)^D}} e^{\frac{-1}{2}(\mathbf{X}-\mu)^T \Sigma^{-1} (\mathbf{X}-\mu)}$$

$$d_M = \sqrt{(x-\mu)^T \Sigma^{-1} (x-\mu)}$$

- Z score and Mahalanobis distance are equivalent

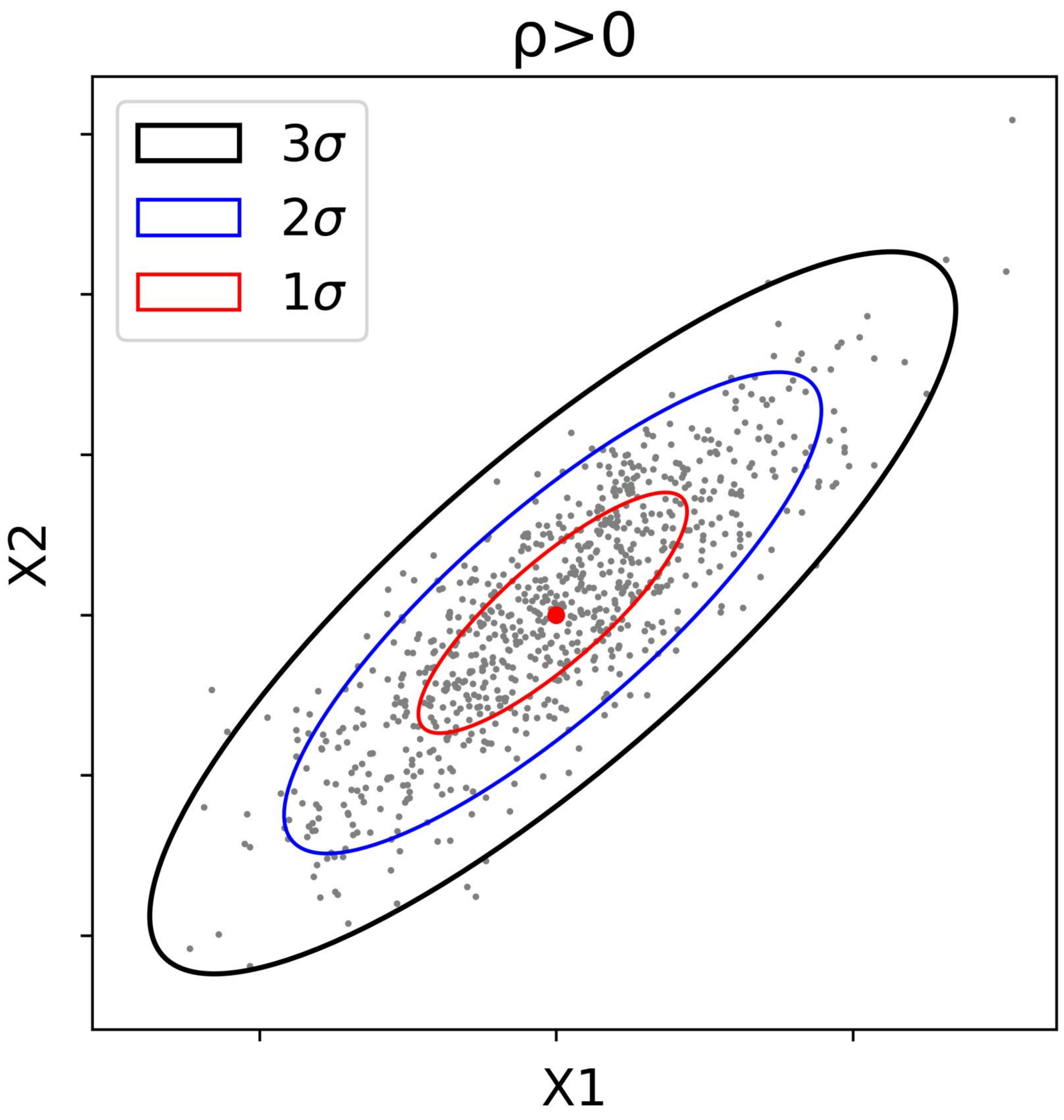
Geometric meaning of contour plots

- Look at Standard deviations in addition to correlation & guess the covariance matrix



- Draw a few more contour plots to familiarize

Geometric meaning of StandardScaler

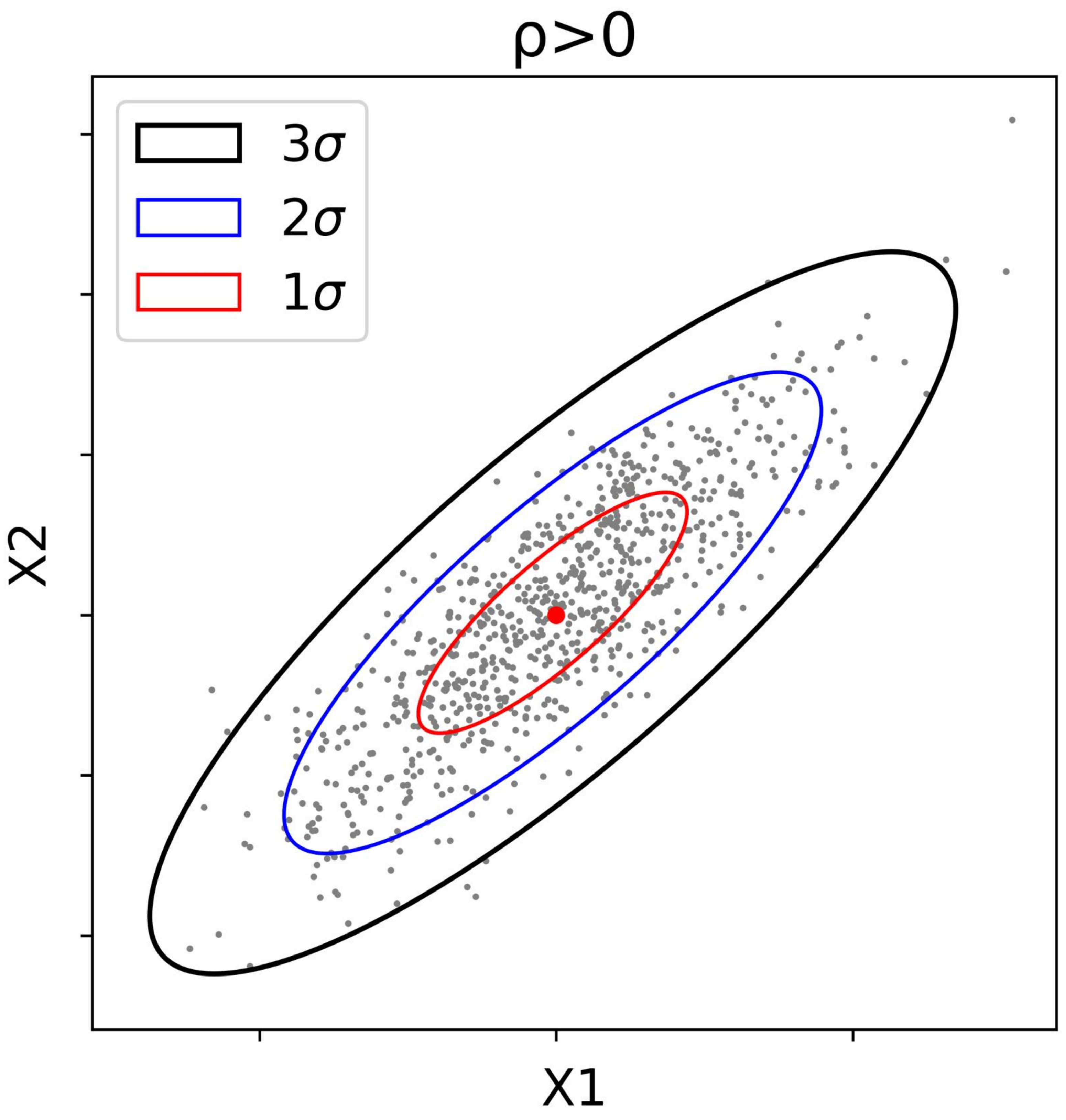


$$\phi(x) = z = \frac{x - \mu}{\sigma}$$

- Demo at https://projector.tensorflow.org/

Back to outlier detection

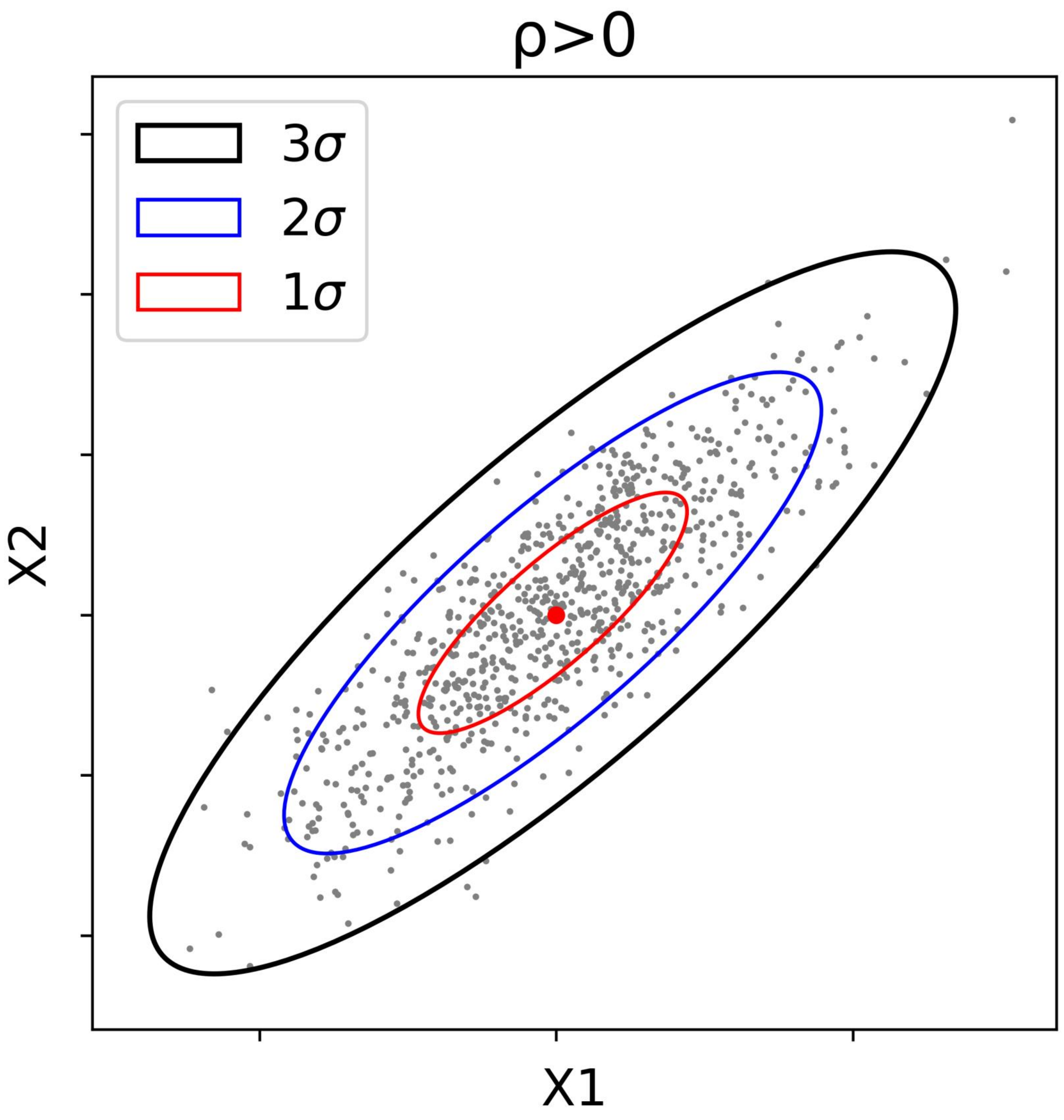
A relook at Mahalanobis distance



- Mark some points and logically see if they are outliers?

$$\sqrt{(\mathbf{X}-\mu)^T\Sigma^{-1}(\mathbf{X}-\mu)}$$

Problems with Mahalanobis distance



- Not robust enough
  - Distribution fitted over all points
  - Add an outlier & distribution "bends" towards it

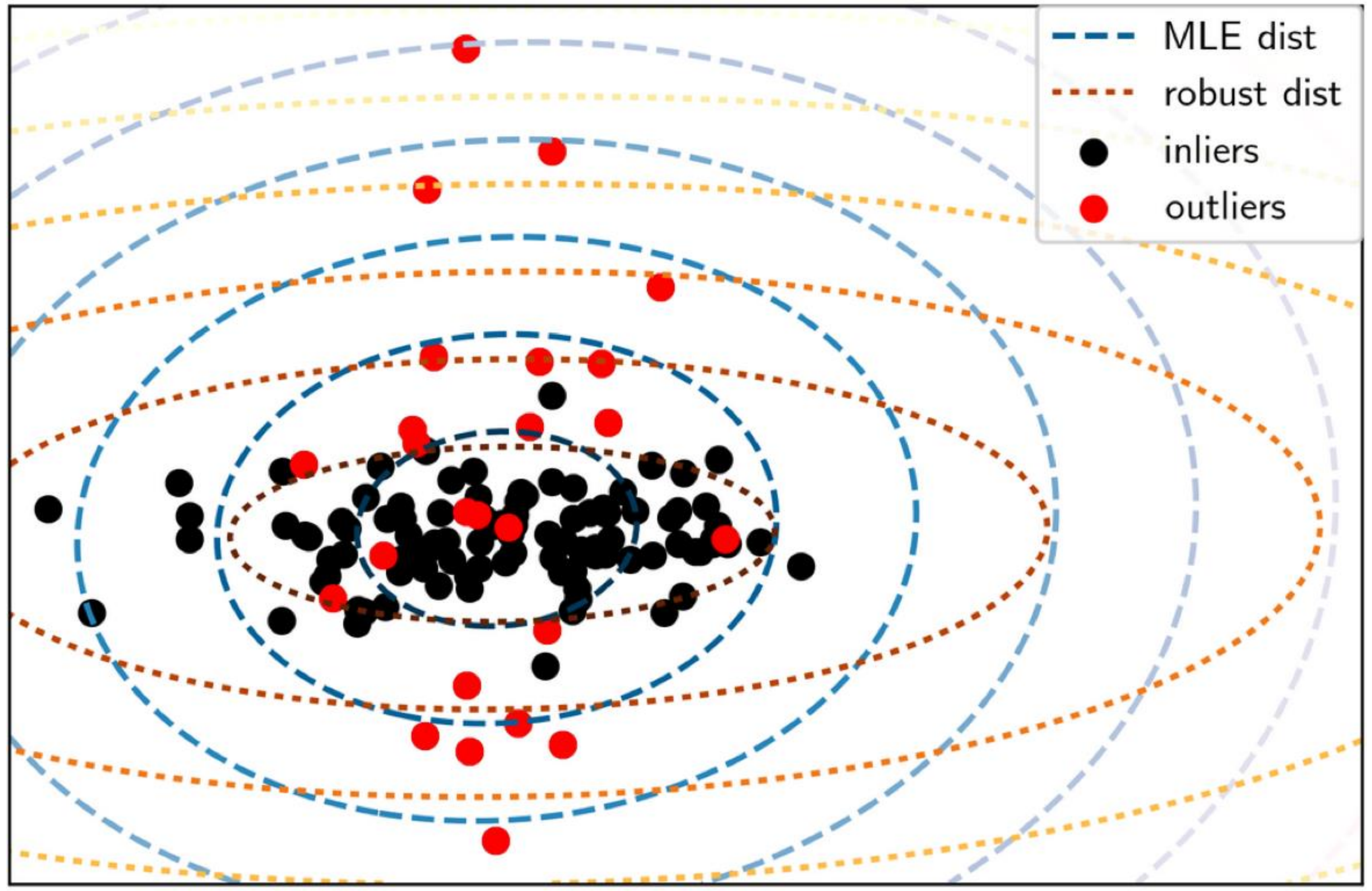
$$\sqrt{(\mathbf{X}-\mu_{MCD})^T\Sigma_{MCD}^{-1}(\mathbf{X}-\mu_{MCD})}$$

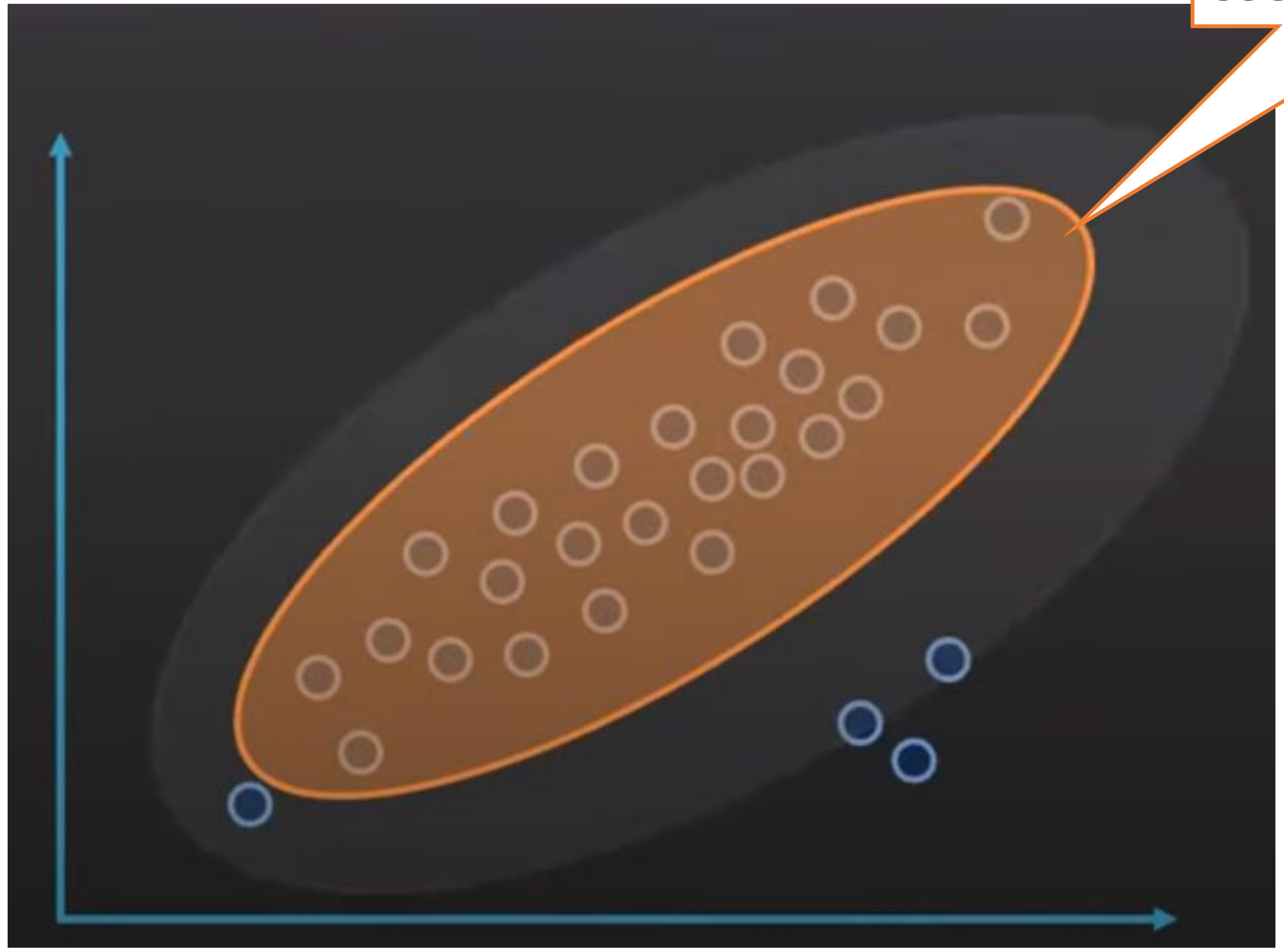
MCD = Minimum Covariance determinant

MCD procedure

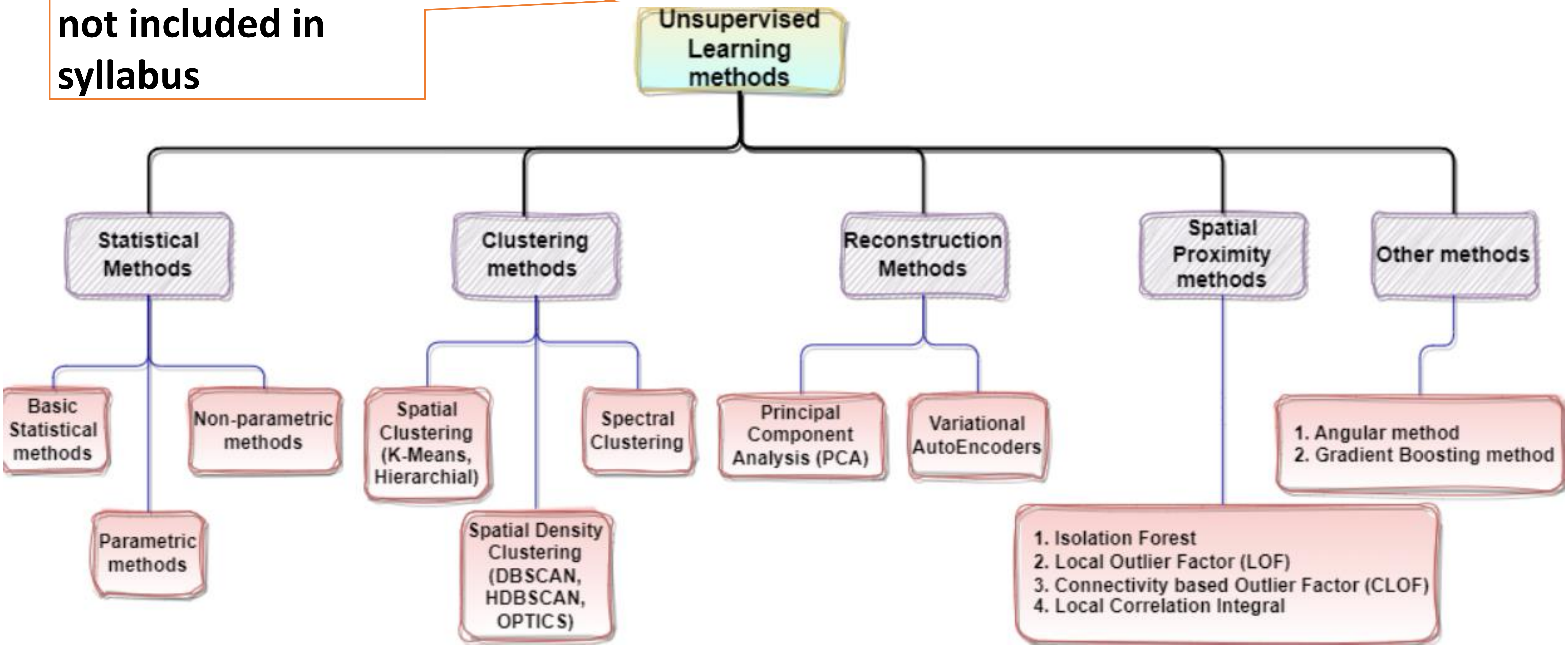
- Take k (typically 0.75 * n) data points
- Sample different data points and find their cov matrix
- Find the cov matrix that has least determinant
- This represents the tightest cloud of points

Elliptic Envelope in sklearn





Optional: This slide not included in syllabus

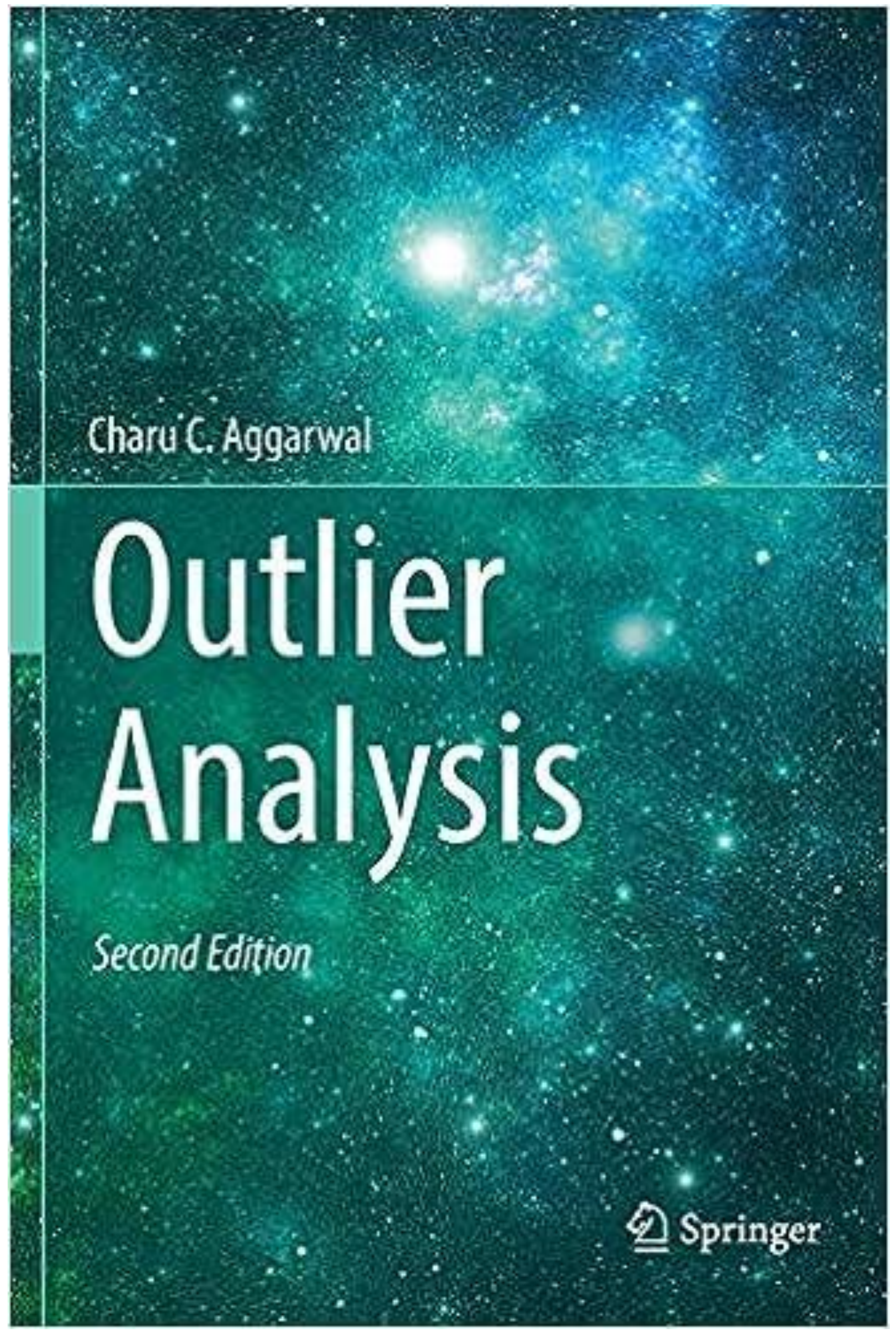


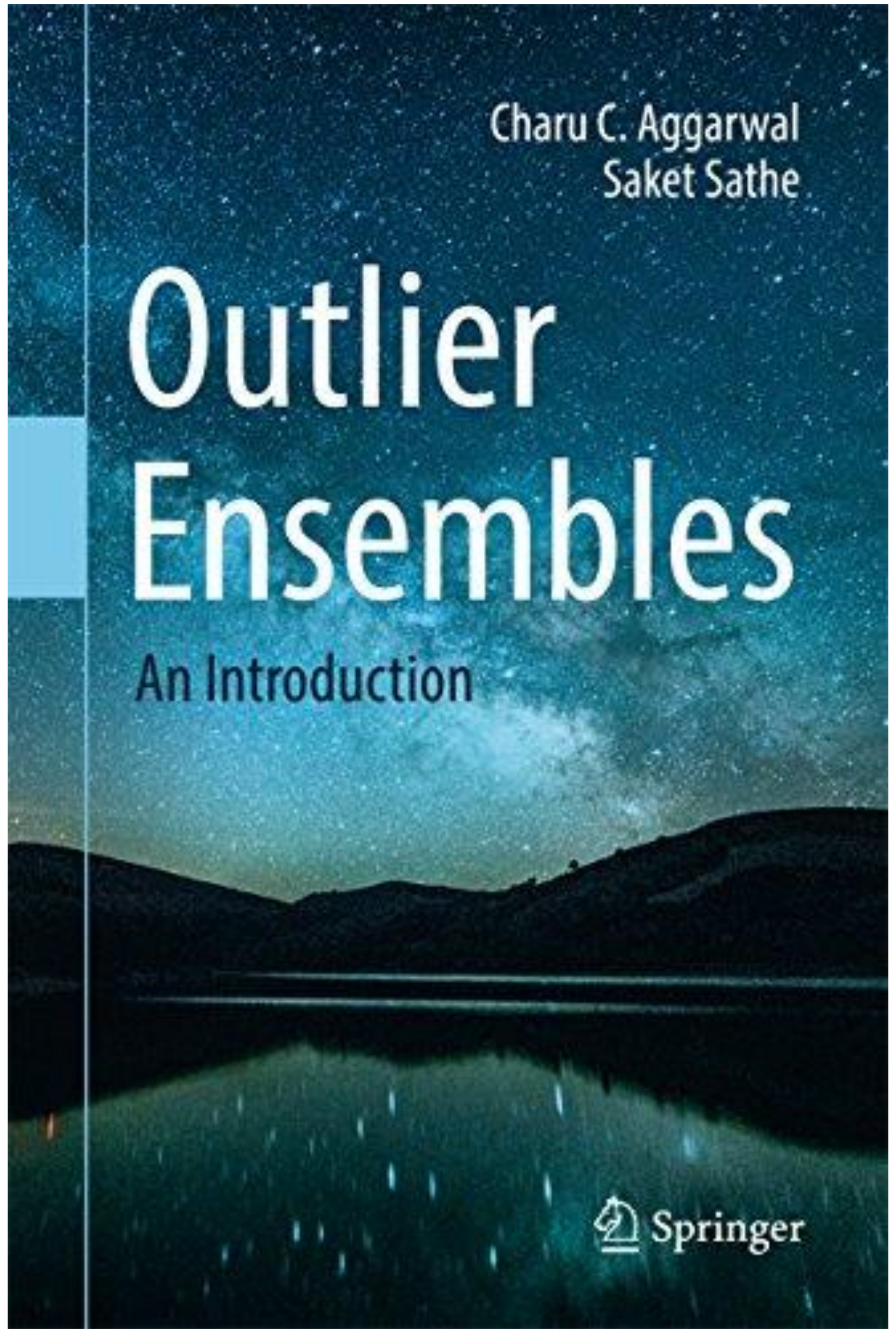
Other outlier detection algorithms (Optional)

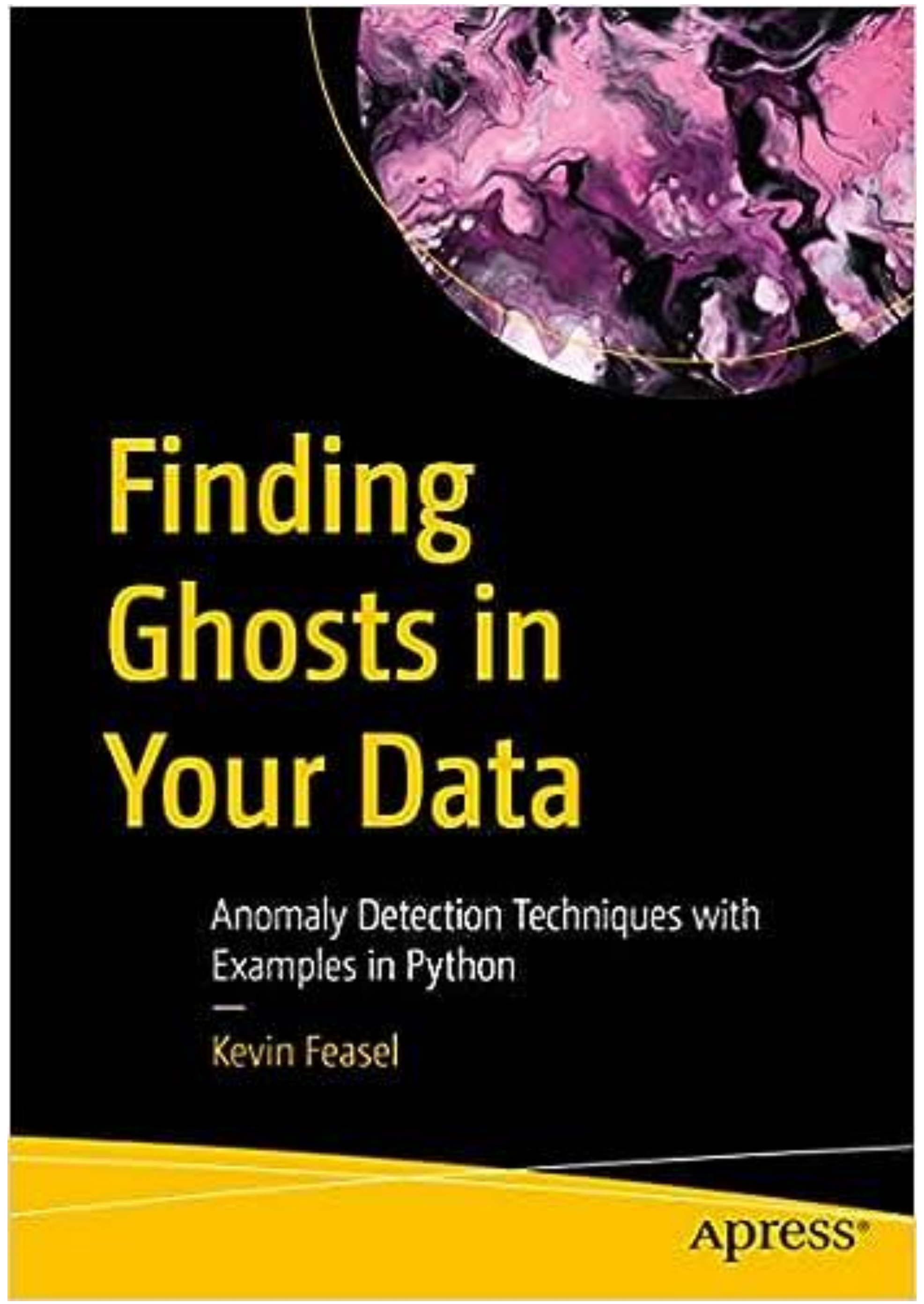
- Proximity based:
  - kNN
  - Isolation Forest, Local Outlier Factor(LOF)
- Clustering based
  - K-Means, Gaussian Mixture Model (GMM) Clustering
- Distance metric based
  - Cook's distance, Gower's distance (mixed data type)
  - MCD on GMM
- Reconstruction based: PCA, Autoencoder
- Take a look at PyOD library

Outlier analysis: Recommended books

- Not part of syllabus. On your own interest



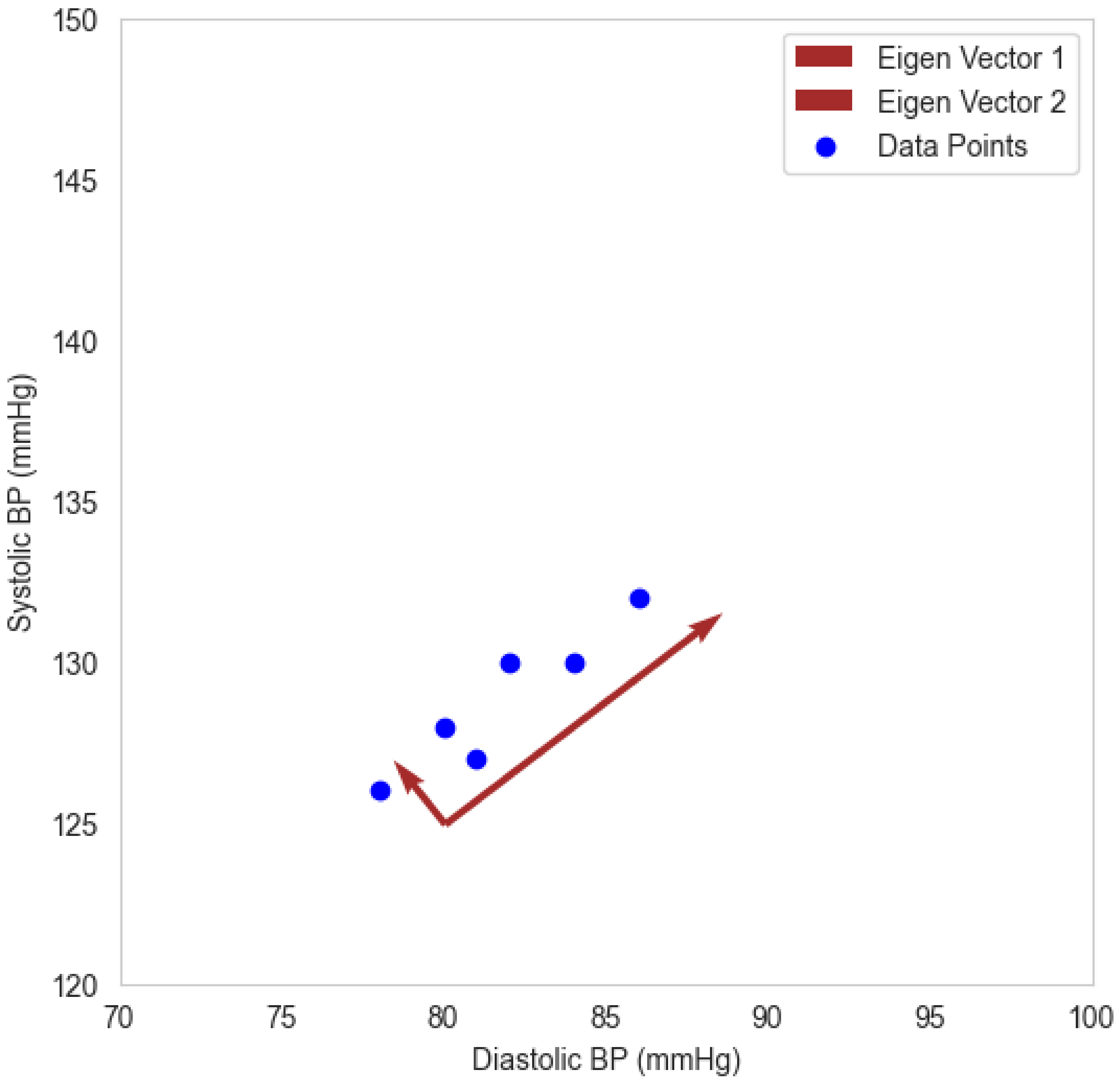




Intuition behind MCD (optional)

Matrix-Vector product & determinant

- Geogebra demo
  - Matrix-Vector product transforms the vector
  - Extent of transformation given by area of parallelogram of original & transformed vectors
  - aka determinant of matrix
- But we are not multiplying data with Cov matrix
- Enter Eigen values of Cov matrix


Eigen Vector 1
Eigen Vector 2
Data Points
150
145
140
135
130
125
120
Systolic BP (mmHg)
70
75
80
85
90
95
100
Diastolic BP (mmHg)

Eigen Values & Vectors

- Eigen values of any matrix represents stretch in direction of vector
- Eigen vector for cov matrix represents direction of max variance
- Product of Eigen values = Determinant of square matrix
- Combine these ideas
  - Determinant is a single measure of spread of data
- As an aside: This determinant-spread relation also answers the question why determinant of cov matrix is in denominator of multivariate gaussian PDF formula


QUESTIONS

Literature Survey