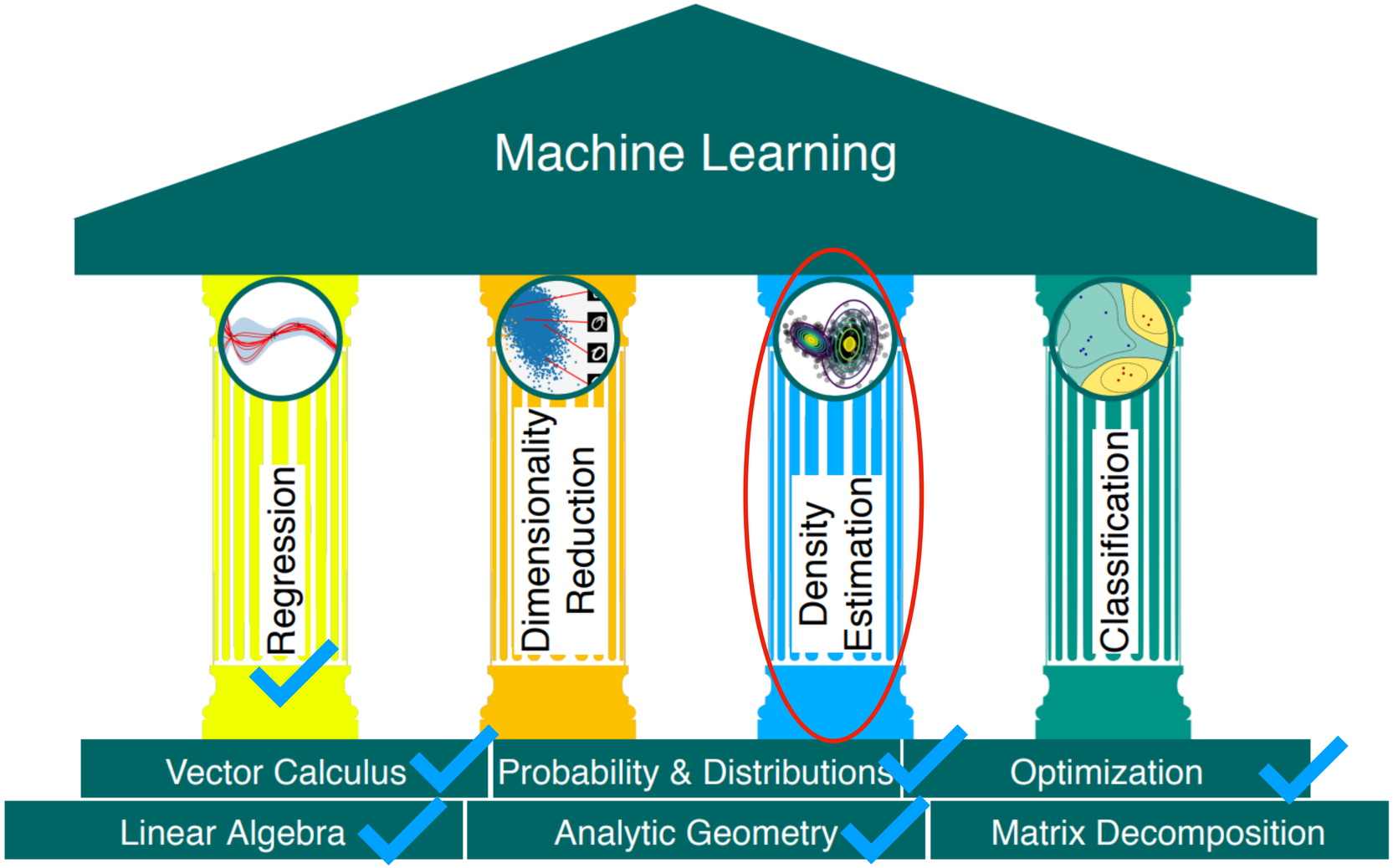
Density estimation with Gaussian mixture models

Week 8 - Introduction to ML / Thang Bui / ANU / 2023 S2

Housekeeping

- Assignment 3 is now available
- [Centrally invigilated, written] exam timetable will be available soon
- Please use Ed!
- Next Monday is a public holiday
  - Lecture: Dunbar Lecture Theatre, Physics Bldg 39A, Thursday 8:30 - 10 am
  - Tutorial: Comp Lab 1.24, Hanna Neumann Bldg 145, Tuesday 5 pm

Foundations of ML



This week:
Density estimation using Gaussian mixture models

Source: Maths for ML Textbook

Recap: Linear regression

Point estimate

$$\theta_{\mathrm{ML}} = (X^\intercal X)^{-1} X^\intercal \mathbf{y} \text{ or } \theta_{\mathrm{MAP}} = (X^\intercal X + N\lambda \mathrm{I})^{-1} X^\intercal \mathbf{y}$$

Exact posterior

$$p(\theta \mid \mathscr{D}) = \mathcal{N}(\theta; \mu, \Sigma)$$

Mean = MAP

$$\mu = \Sigma \sigma^{-2} \mathbf{X}^\intercal \mathbf{y}$$

$$\Sigma = (\sigma^{-2} \mathbf{X}^\intercal \mathbf{X} + \sigma_o^{-2} \mathrm{I}_D)^{-1}$$

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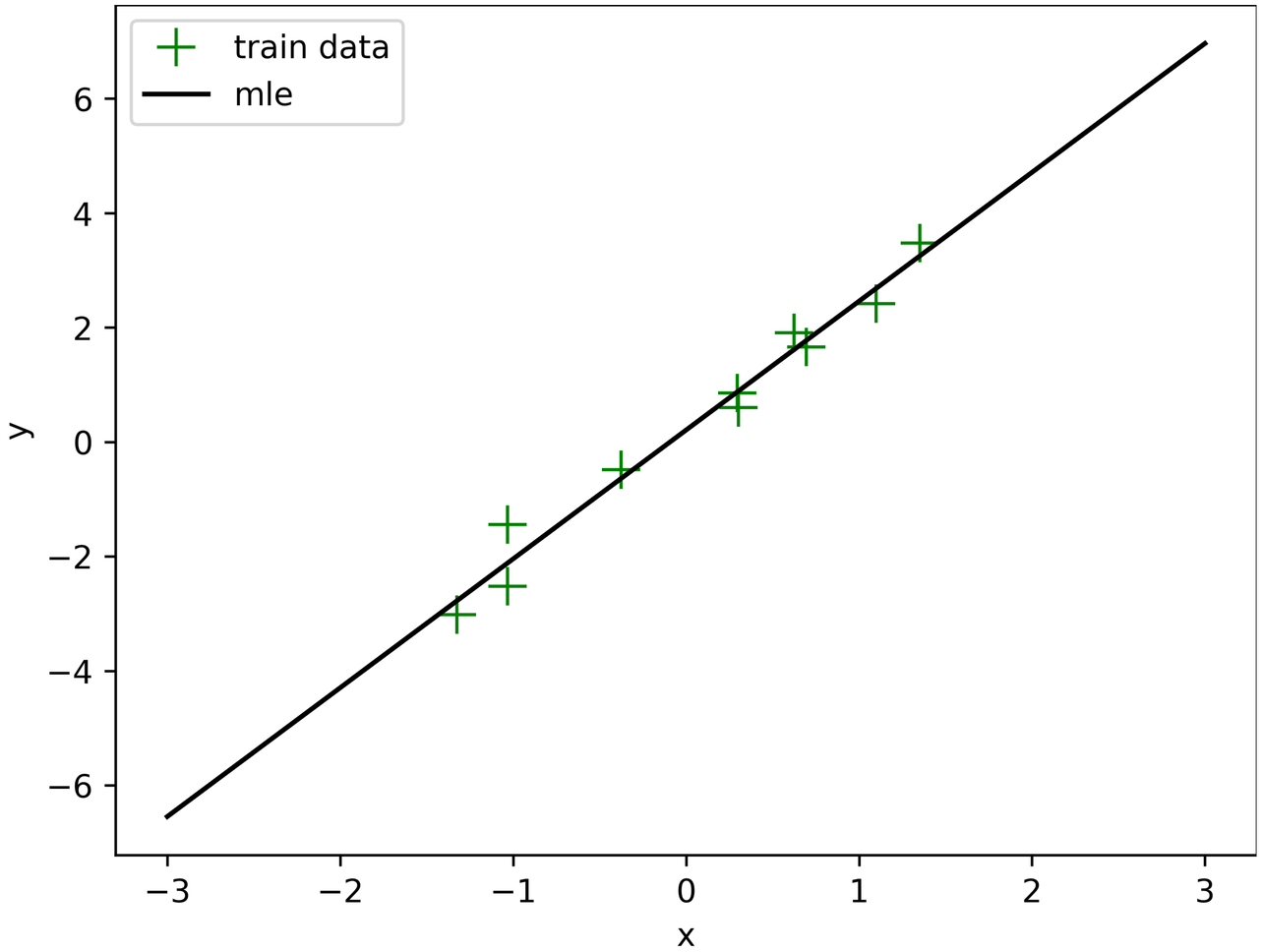

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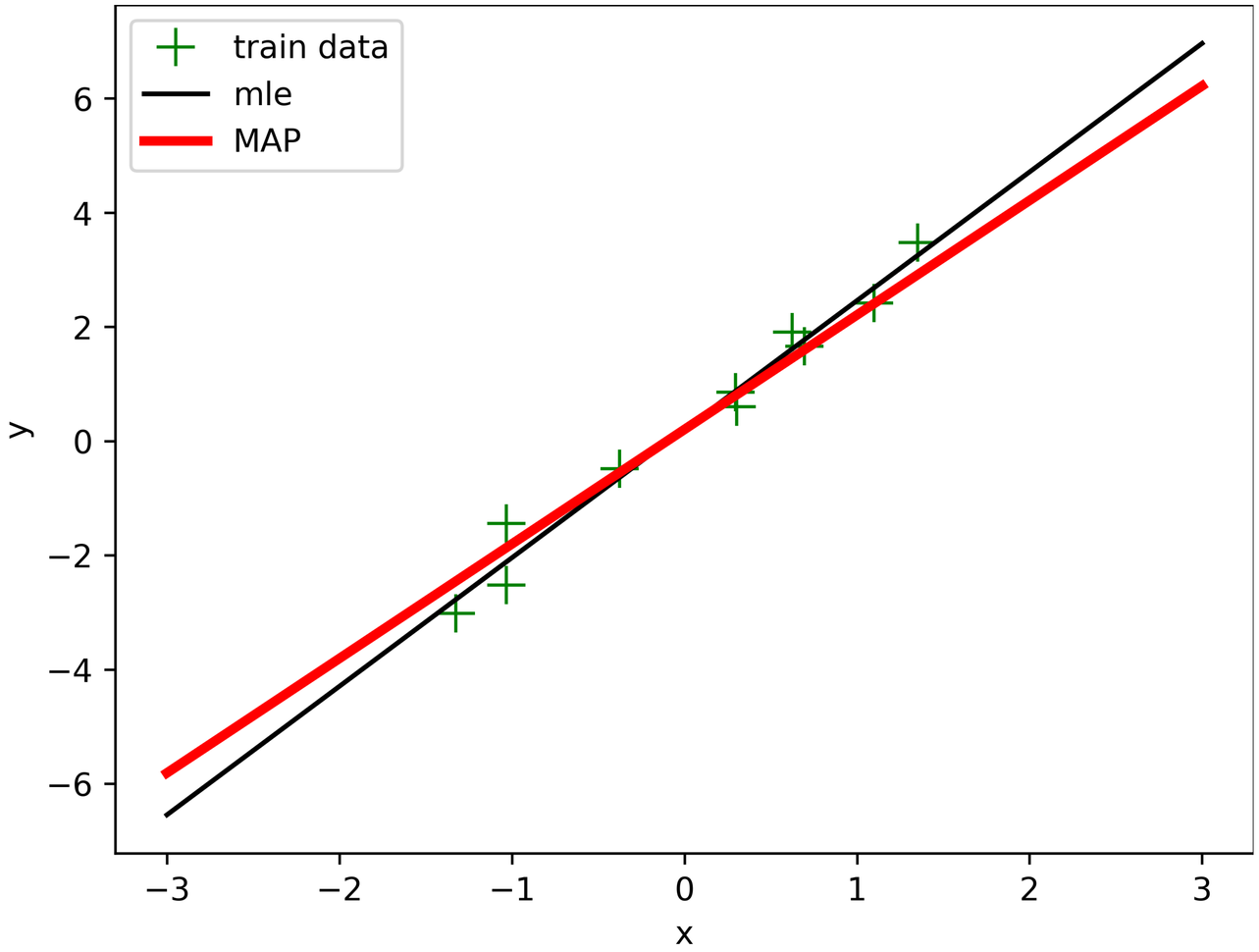

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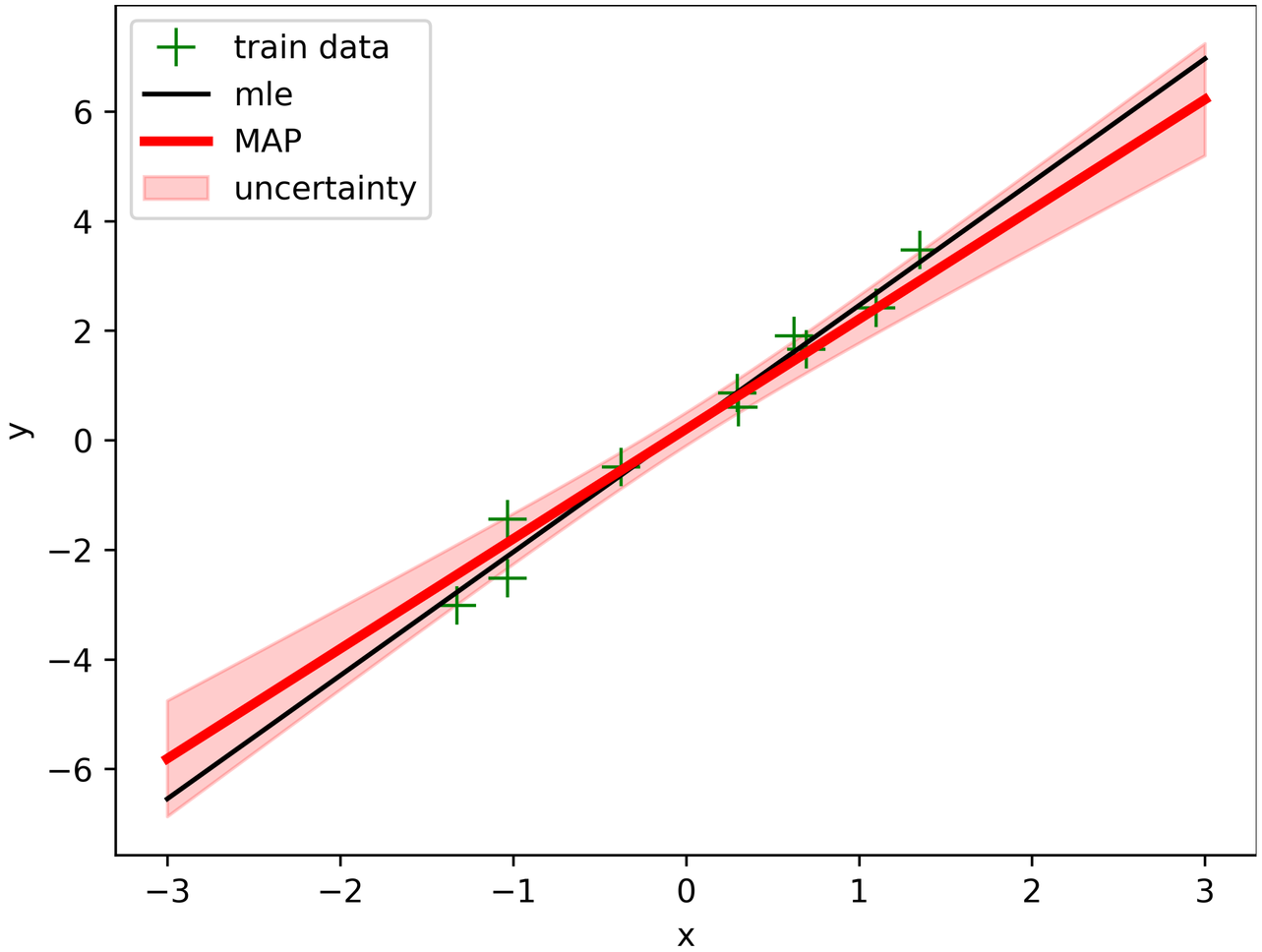

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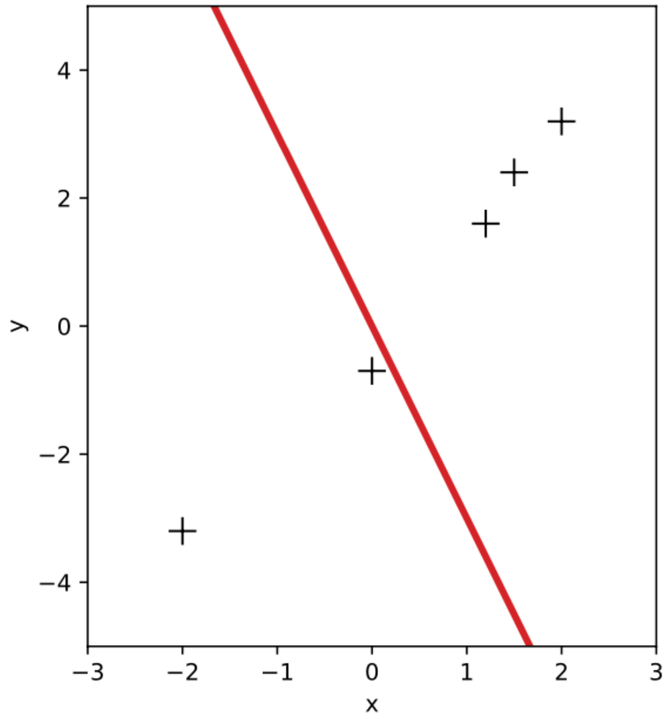

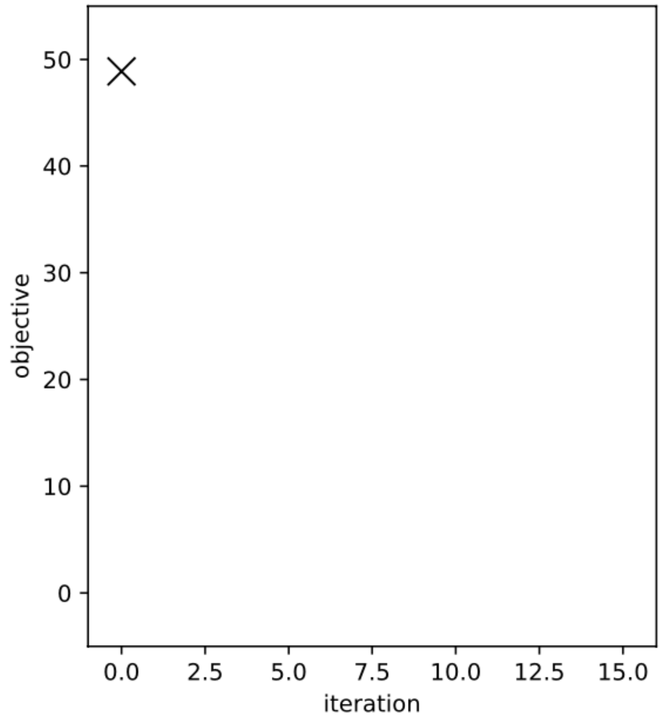

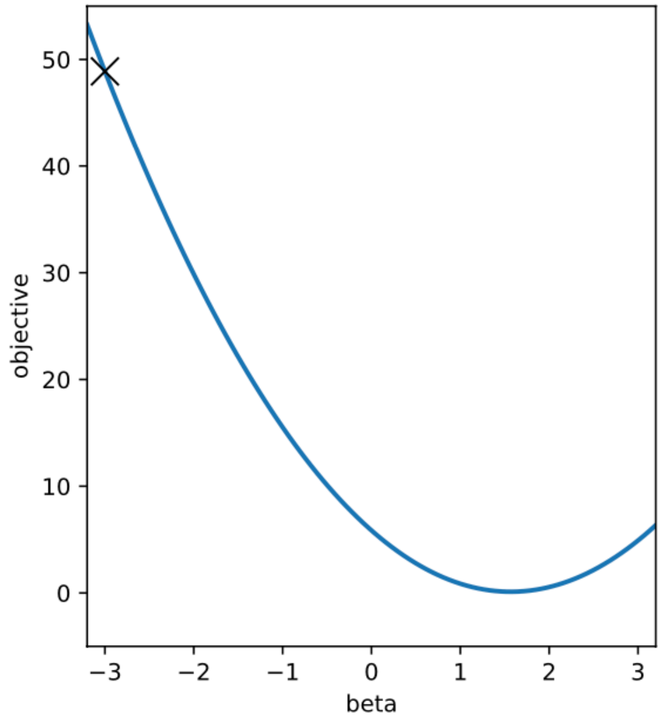

Another example: https://playground.tensorflow.org/

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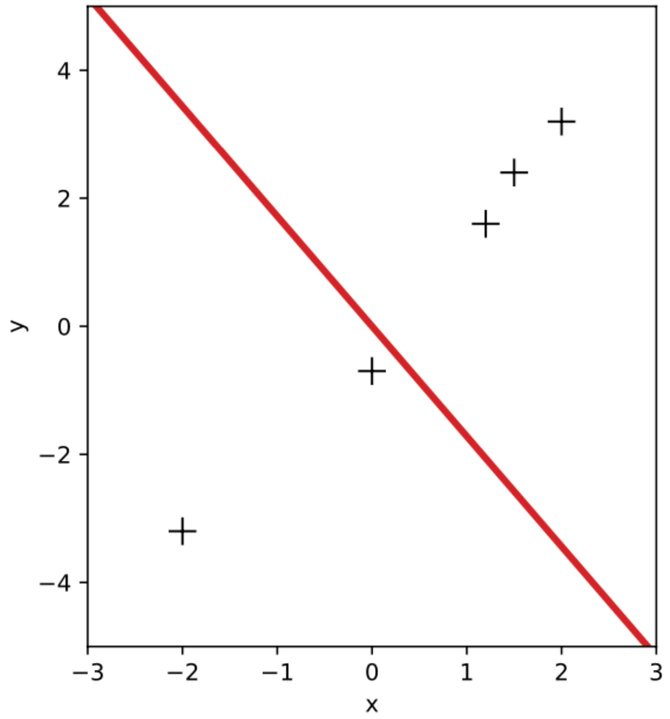

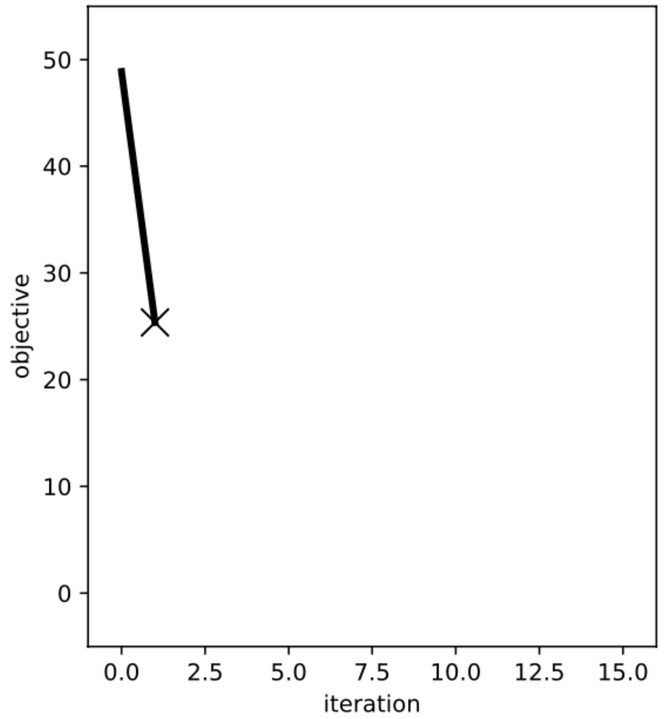

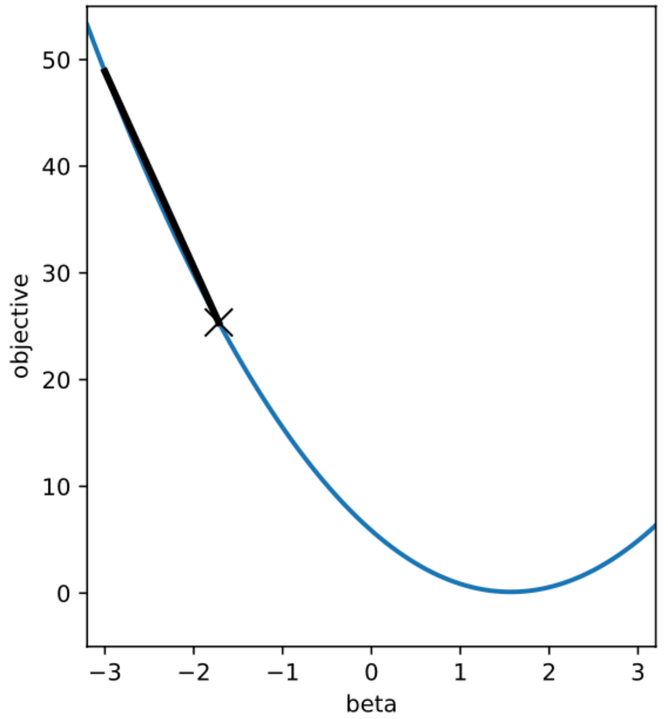

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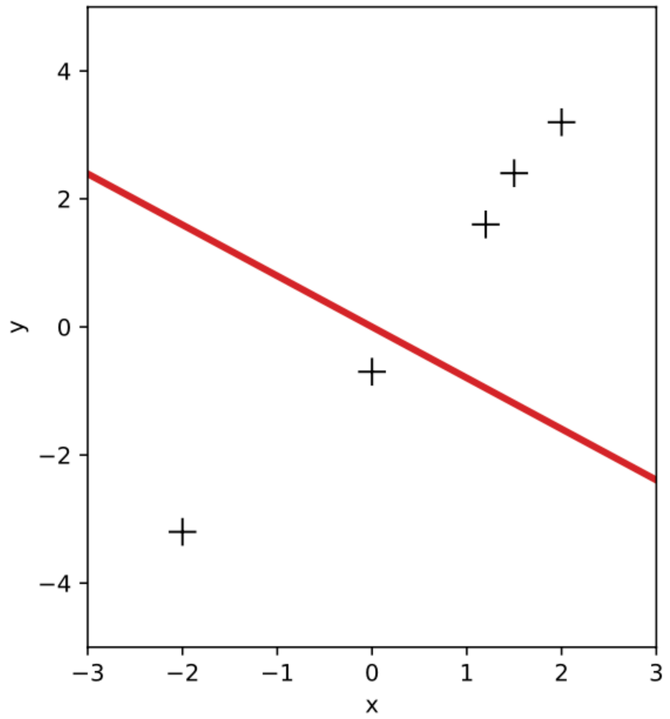

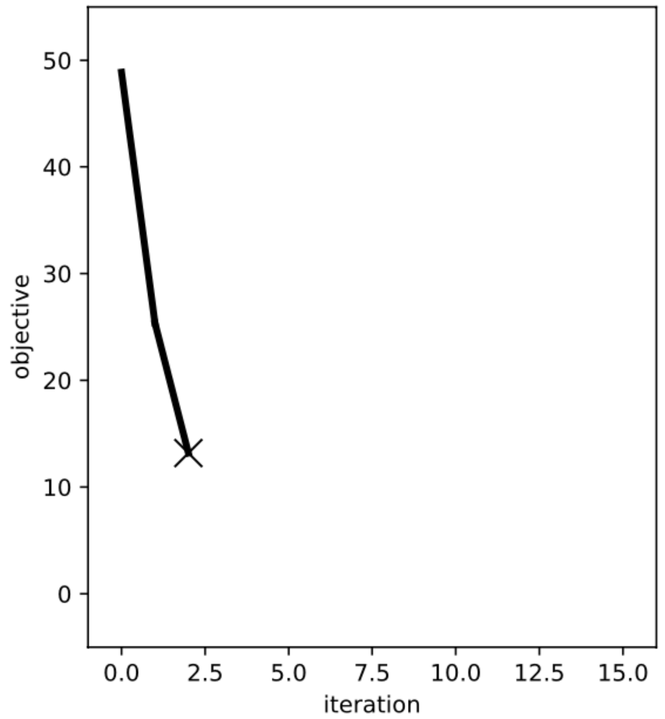

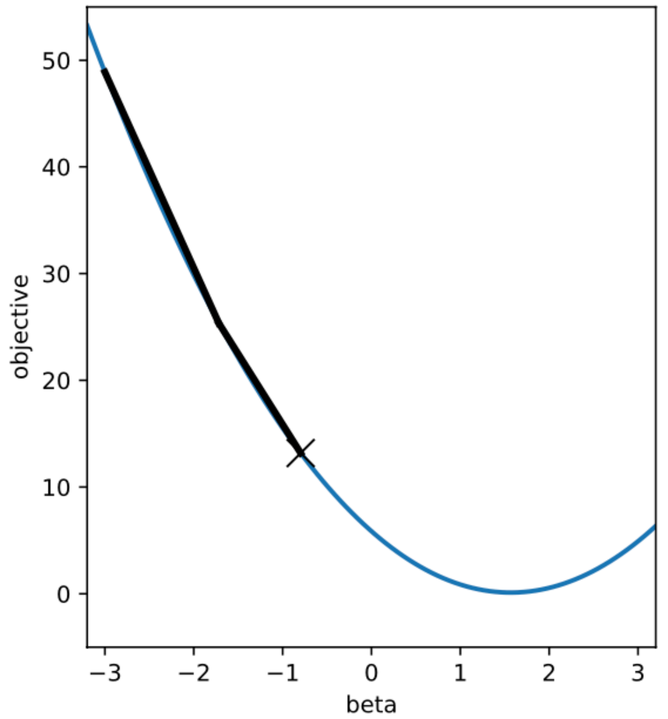

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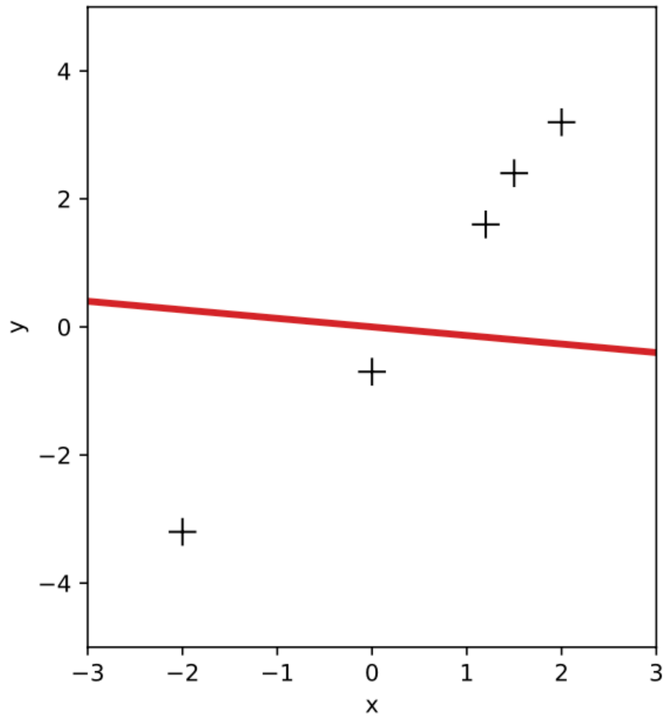

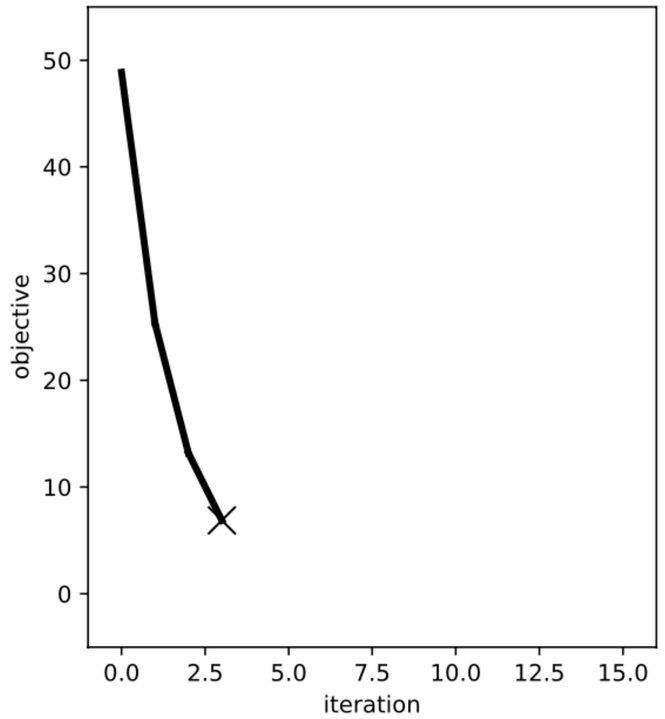

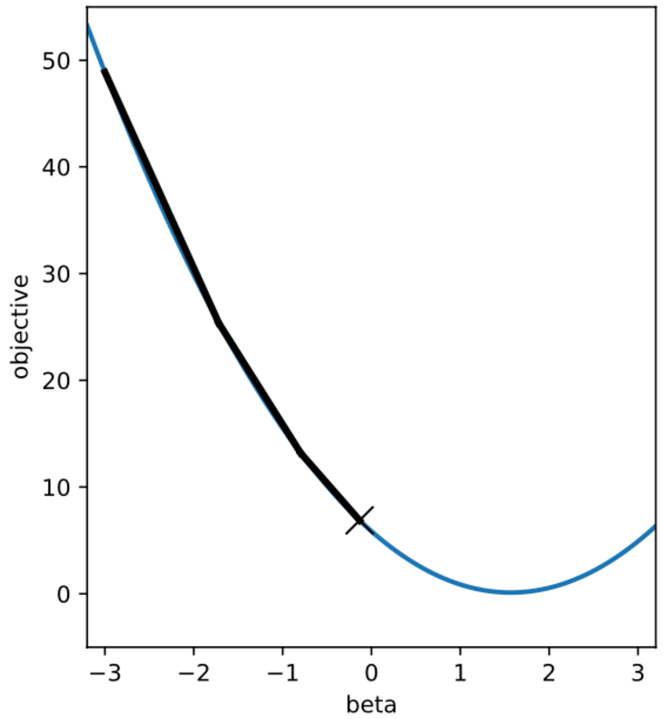

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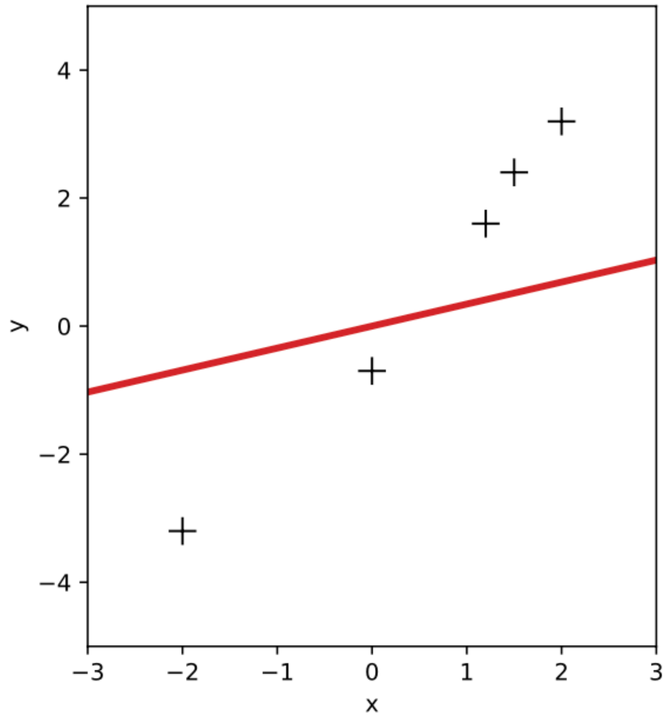

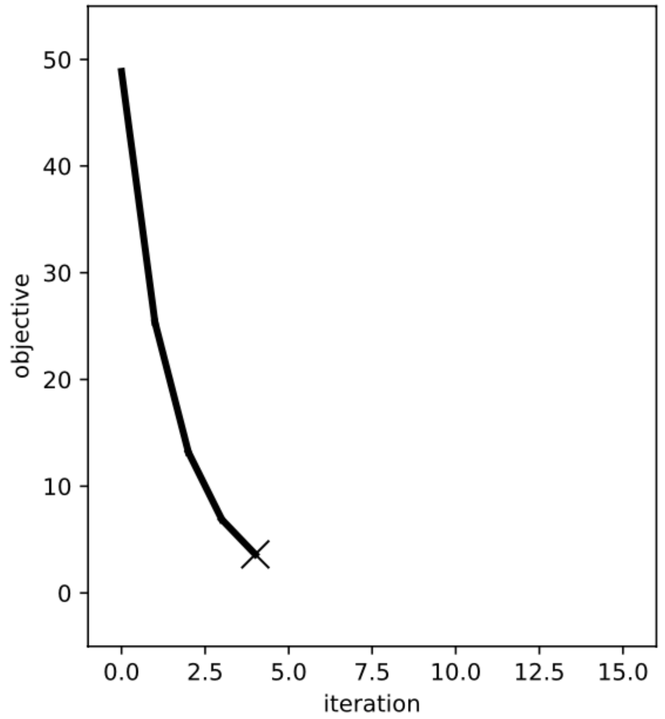

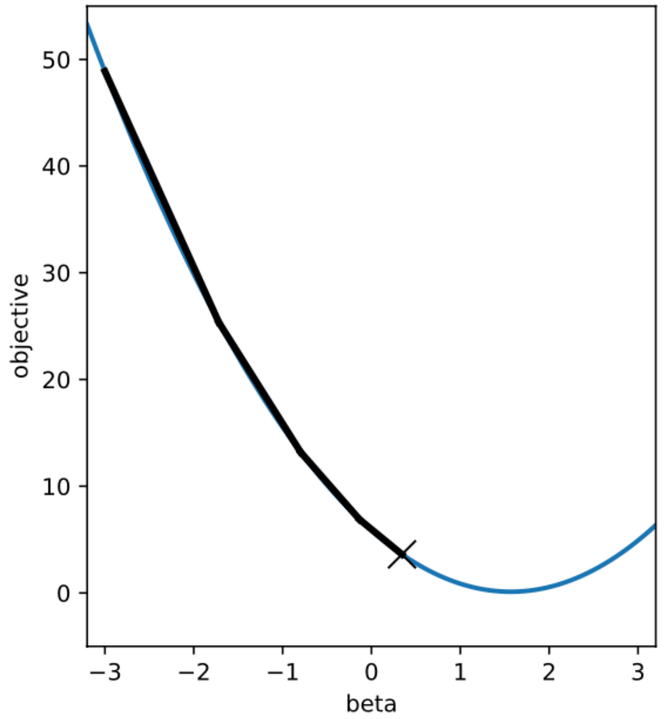

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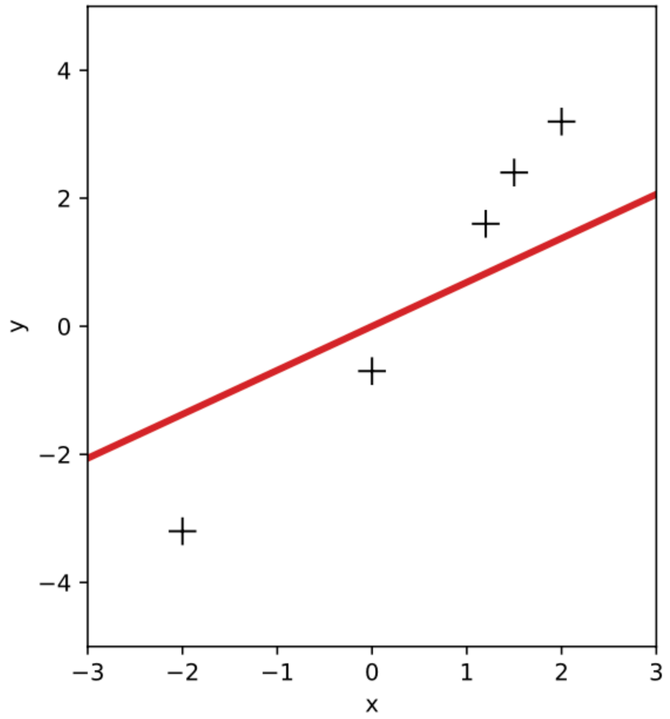

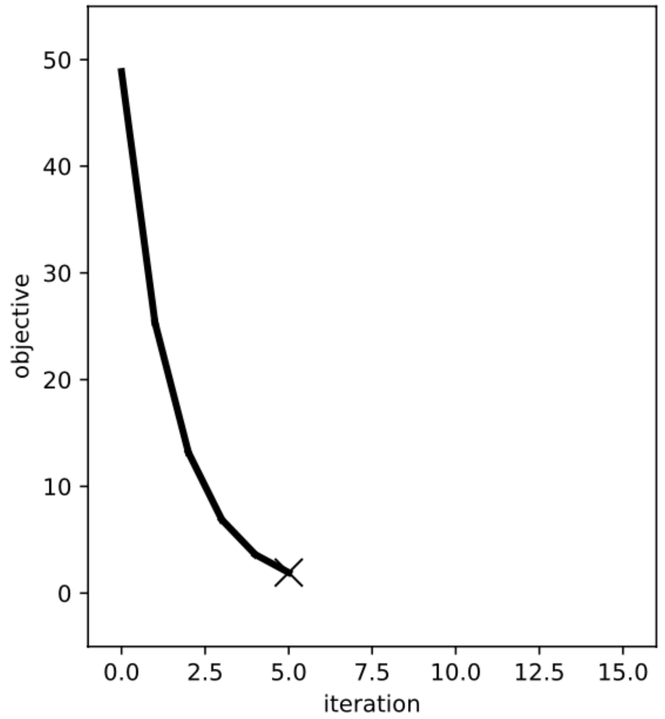

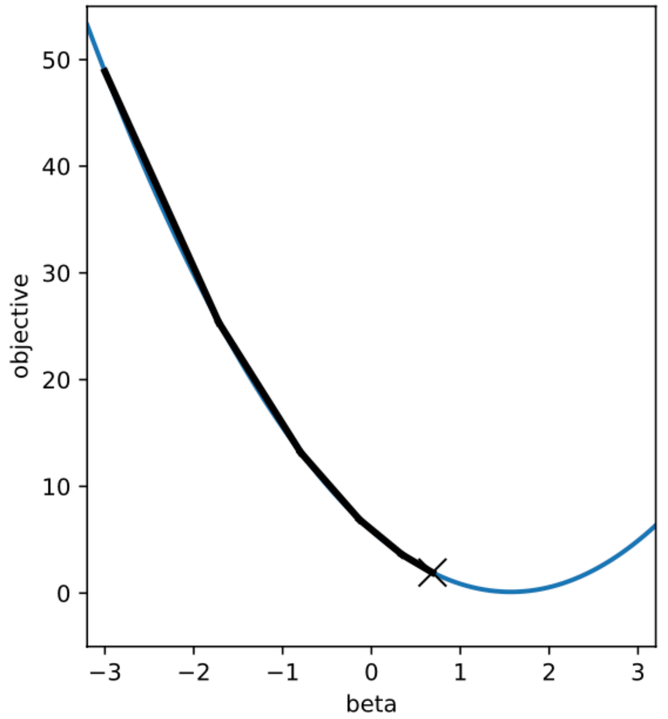

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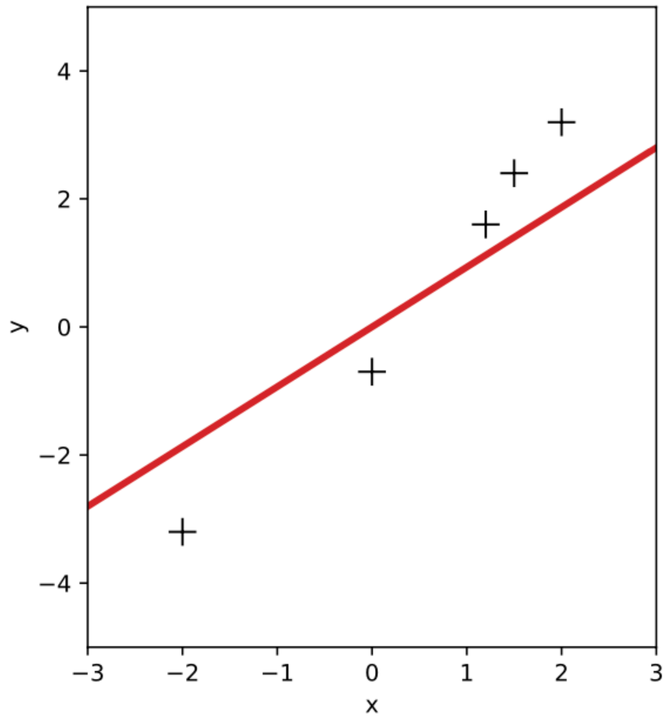

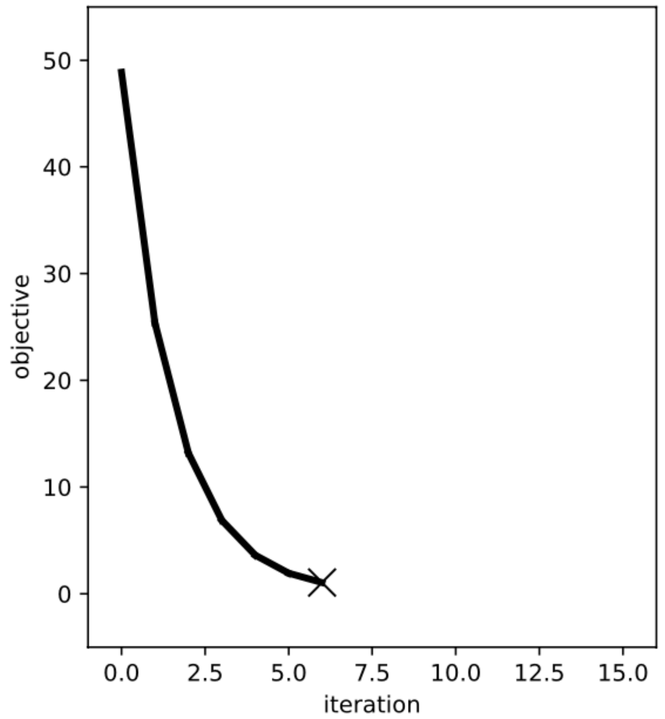

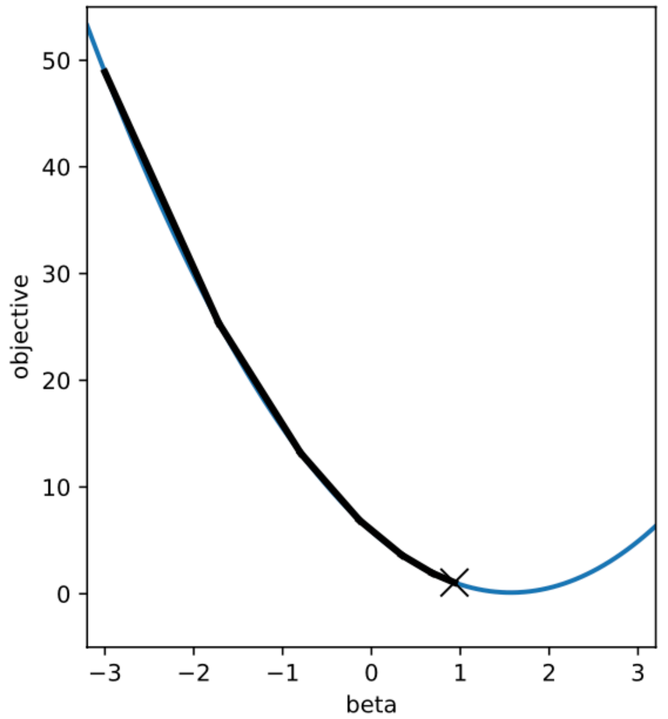

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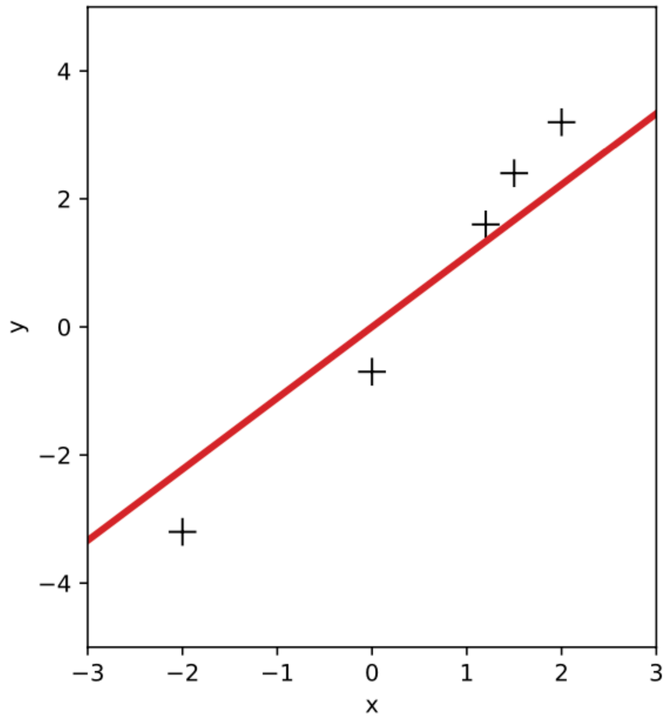

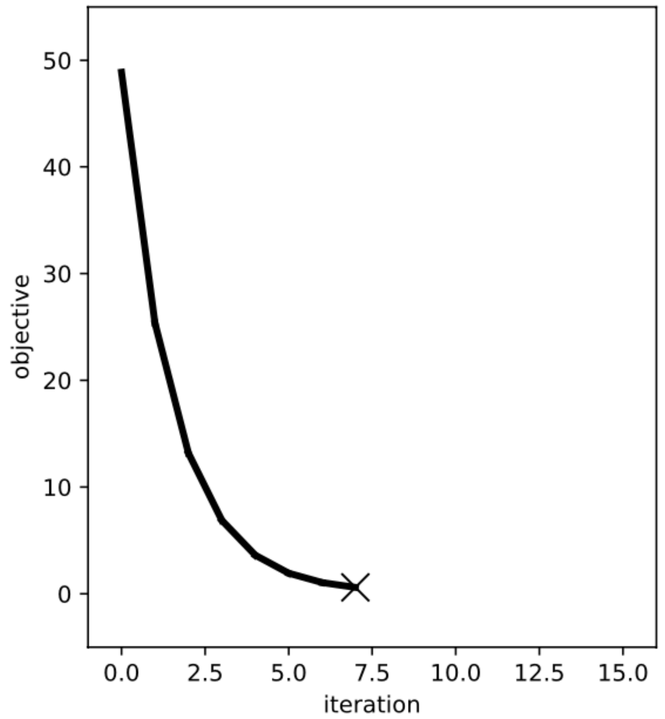

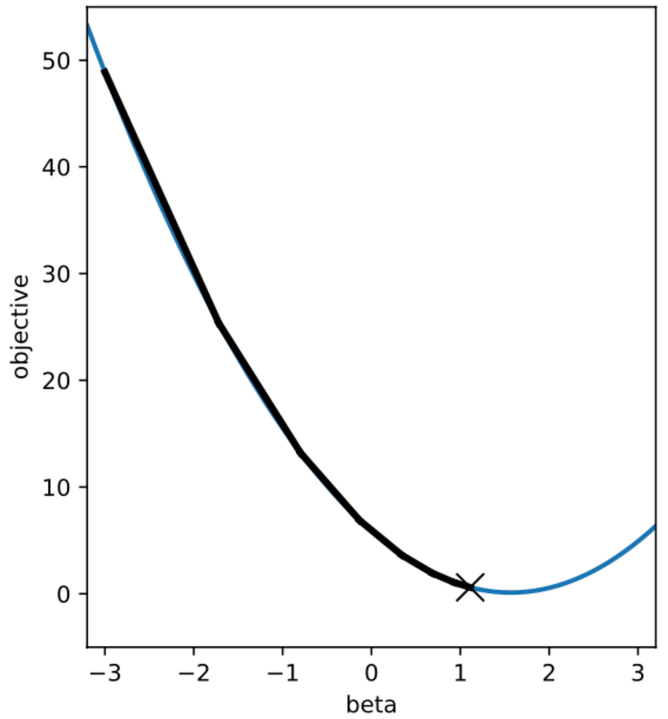

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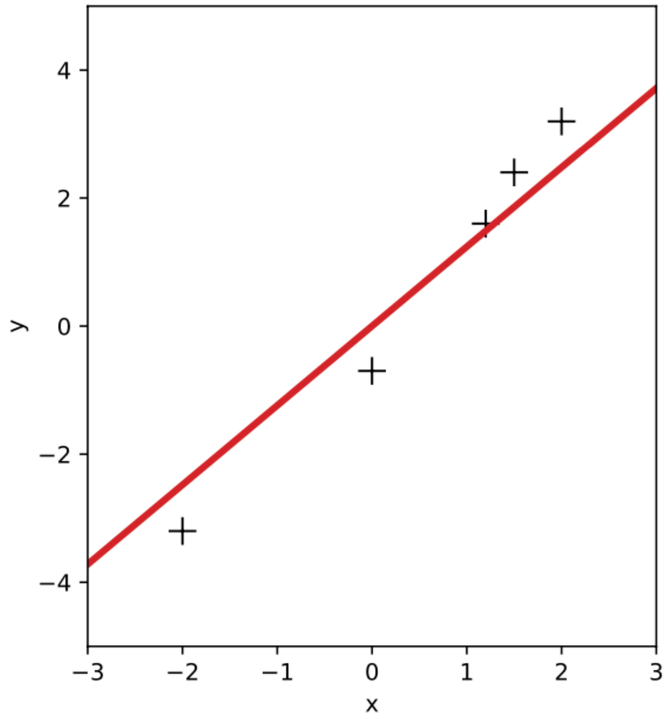

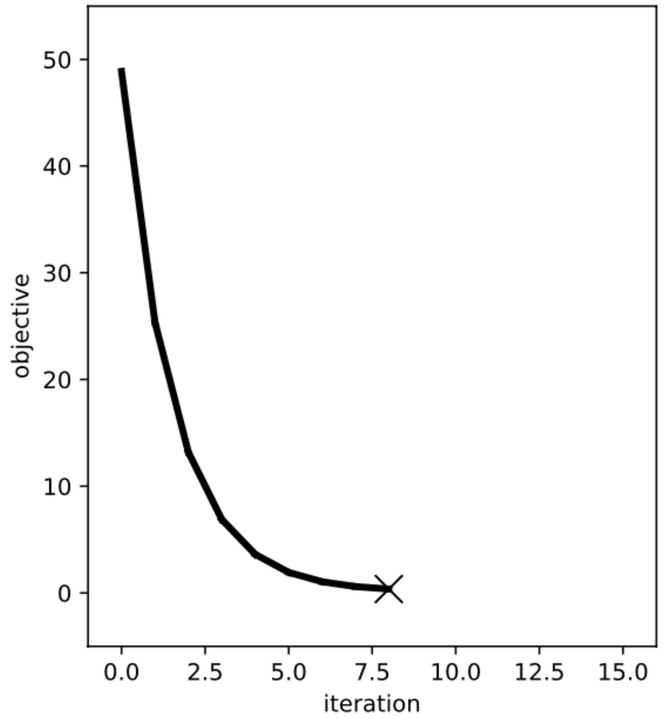

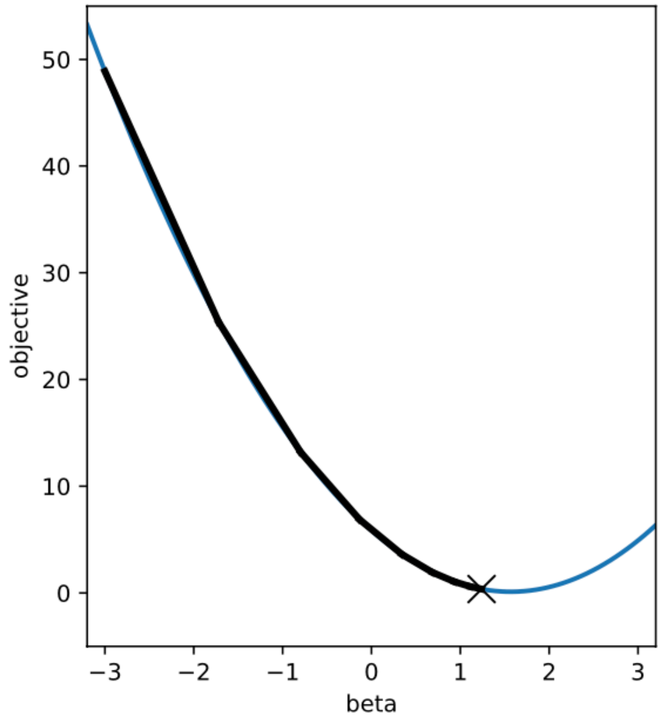

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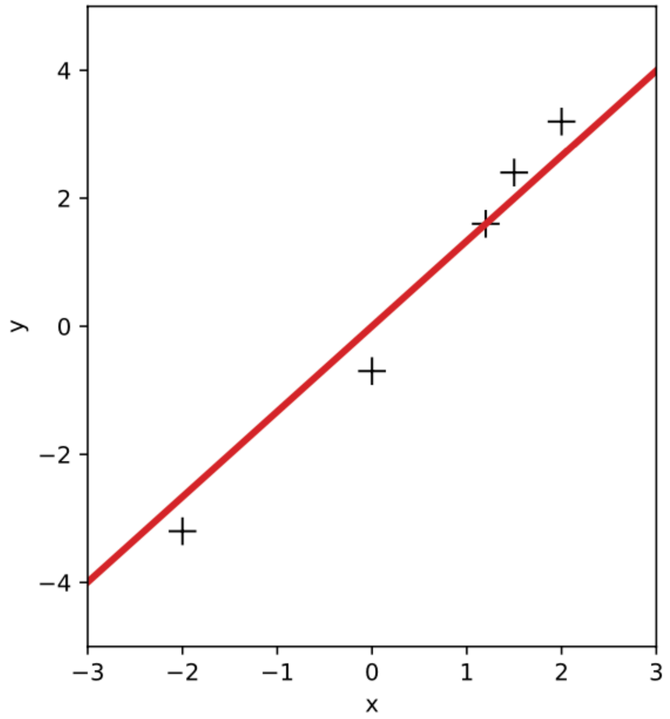

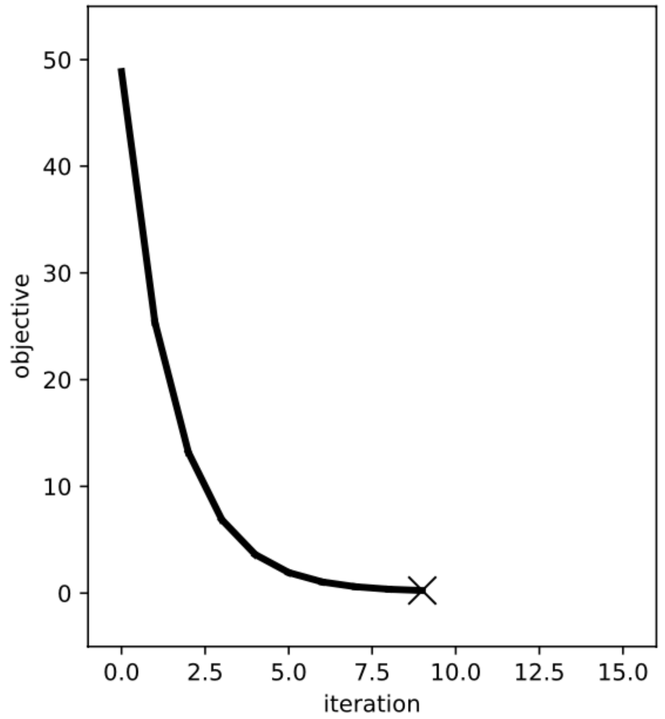

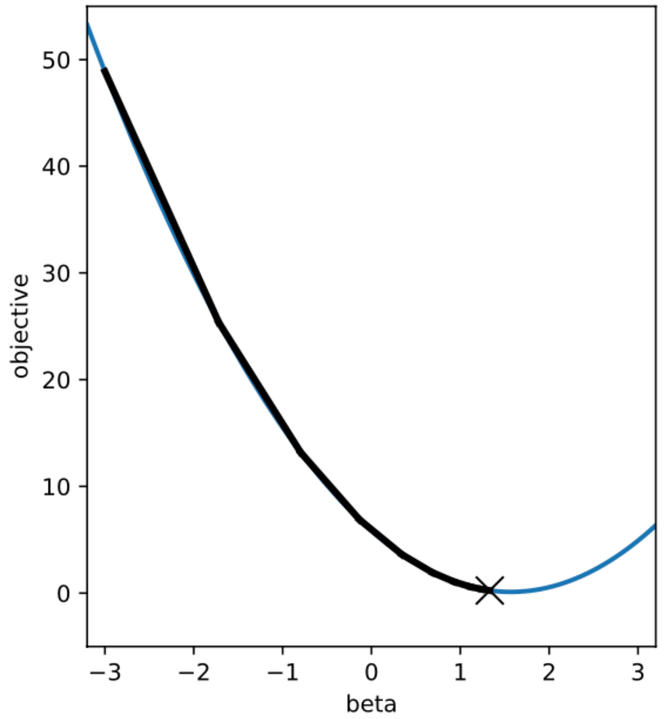

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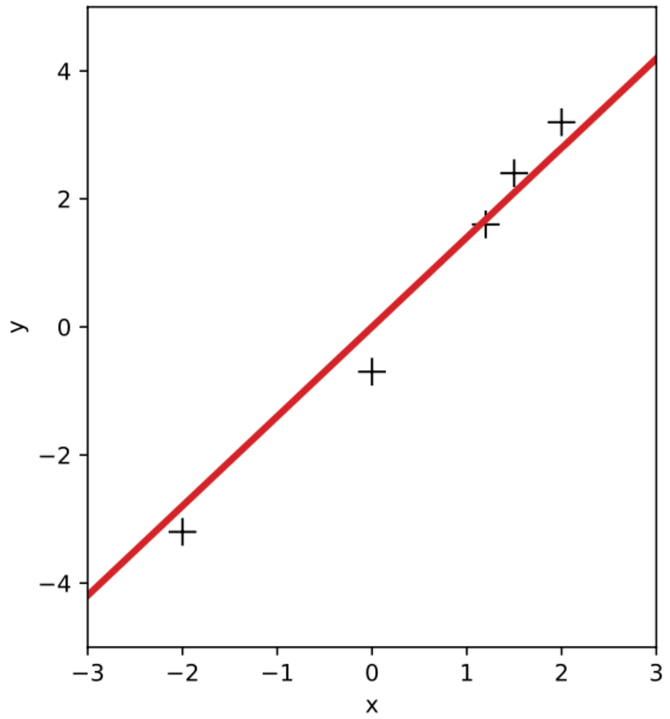

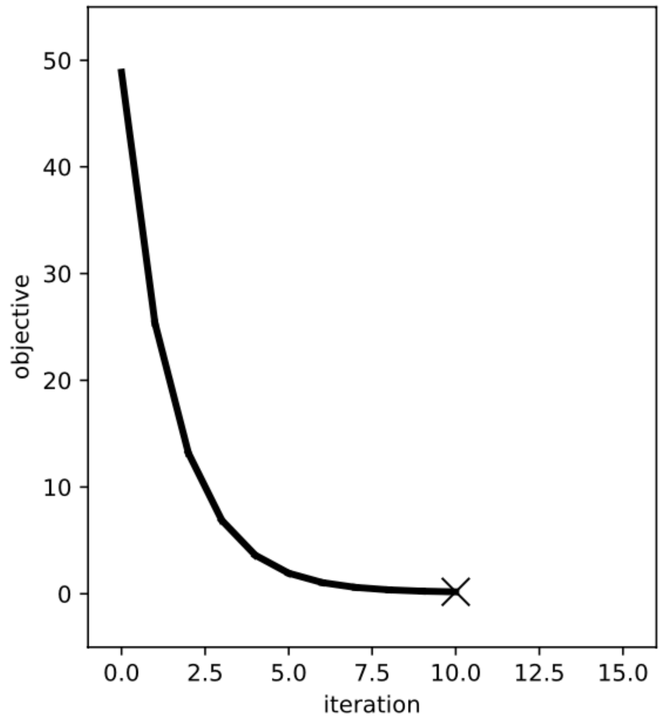

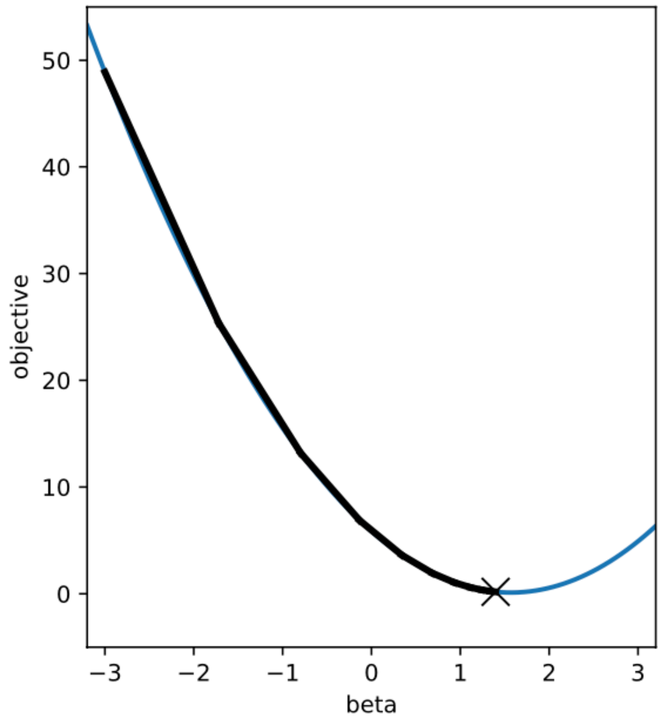

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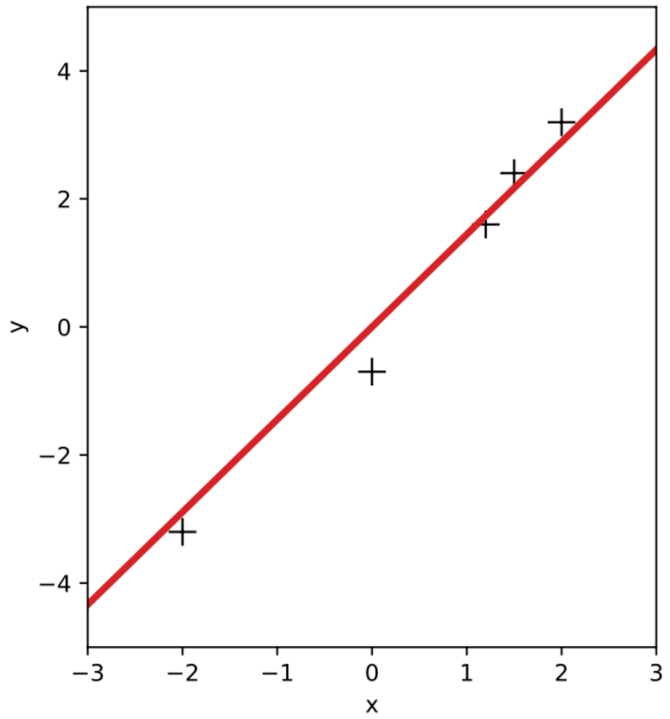

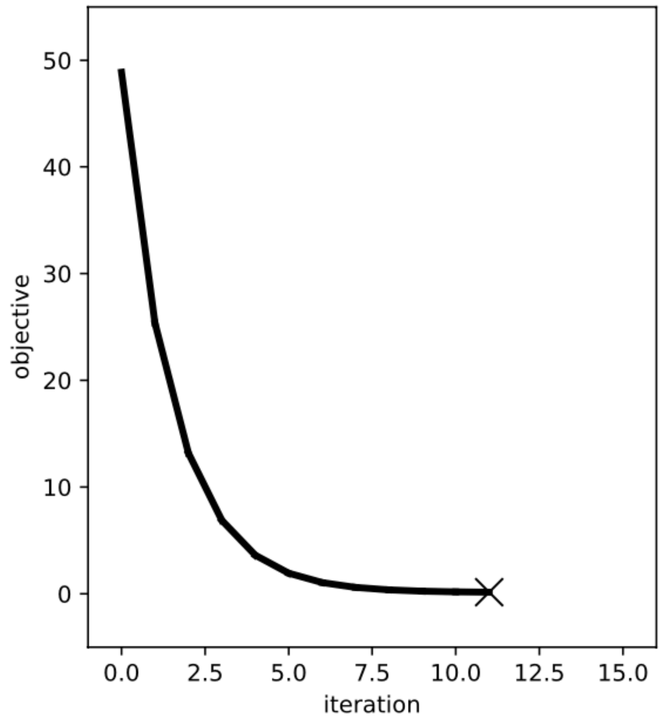

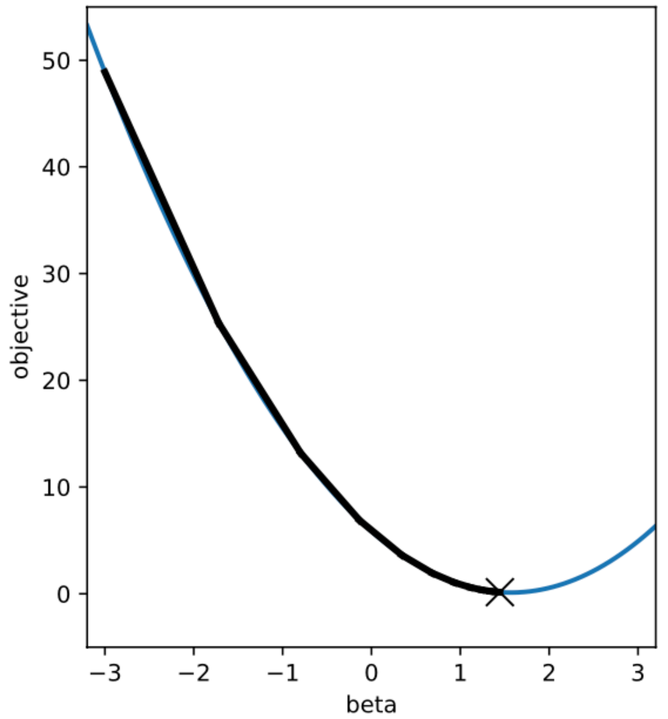

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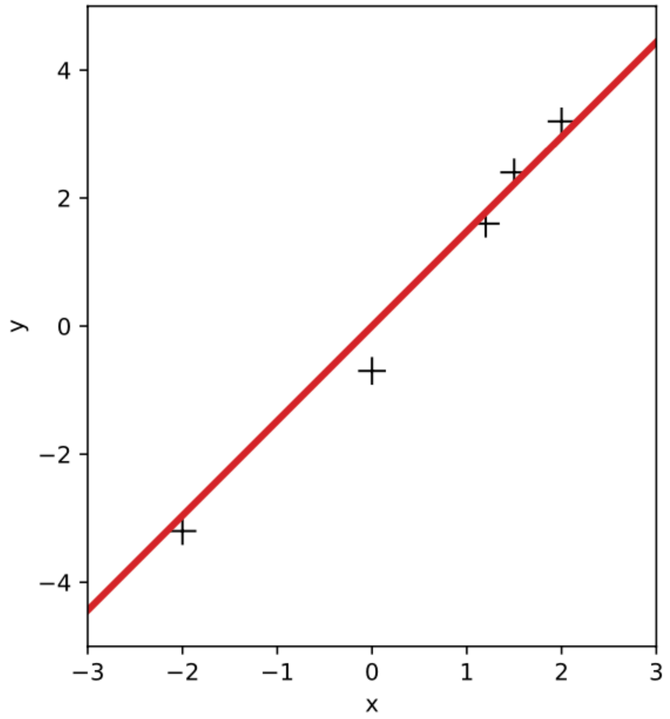

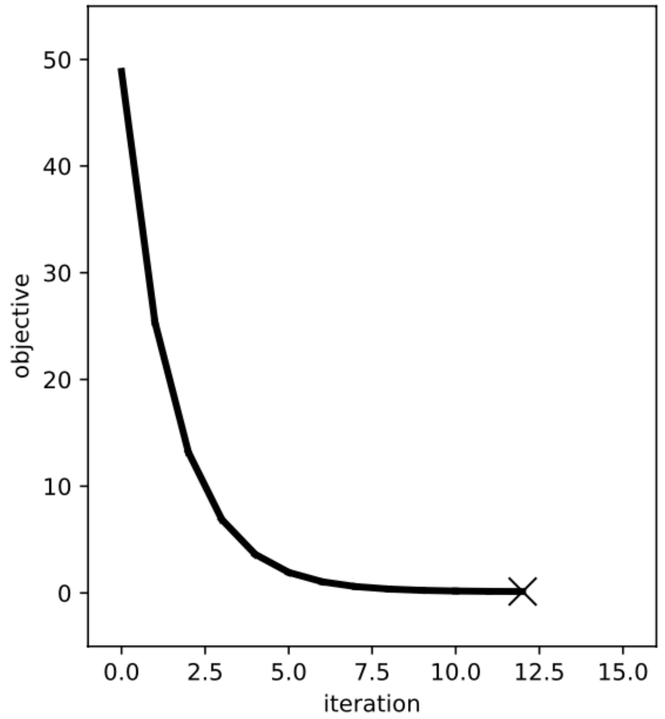

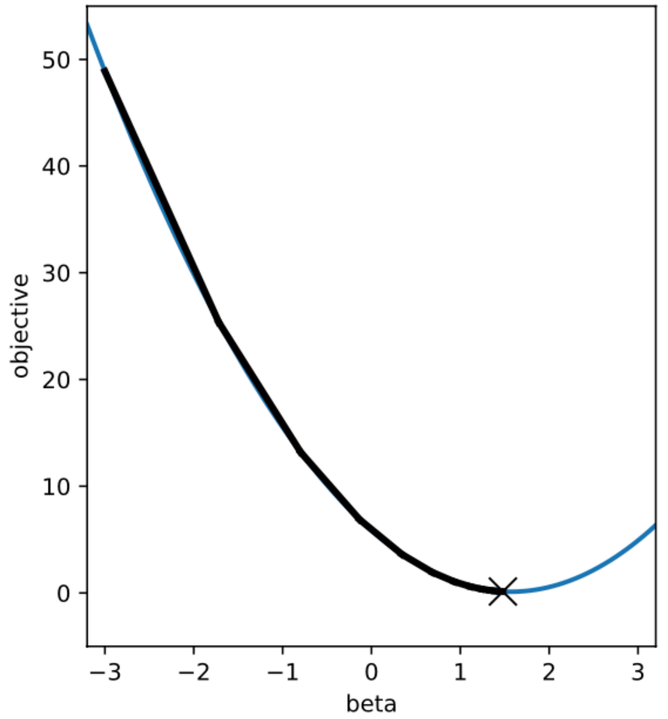

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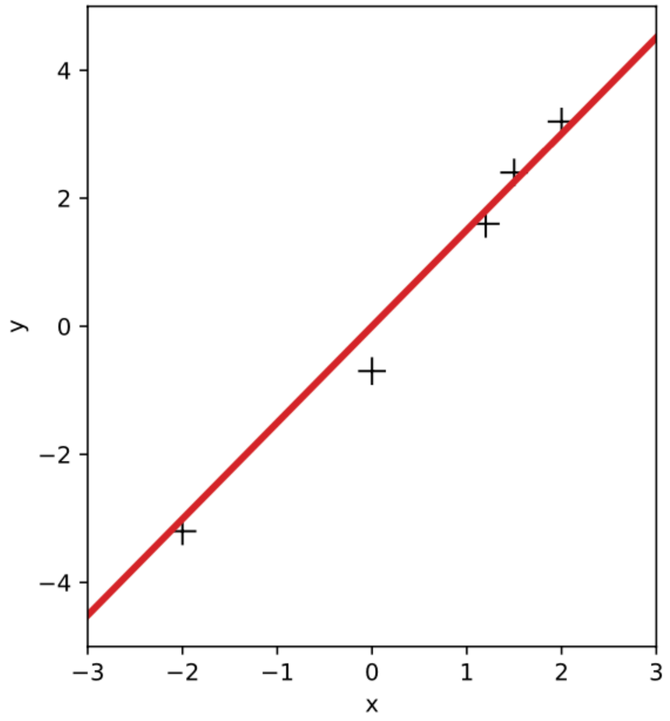

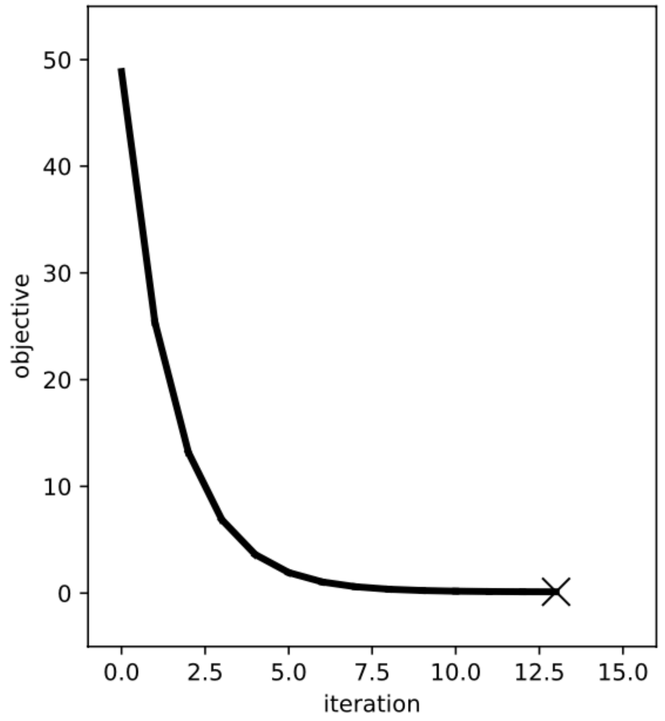

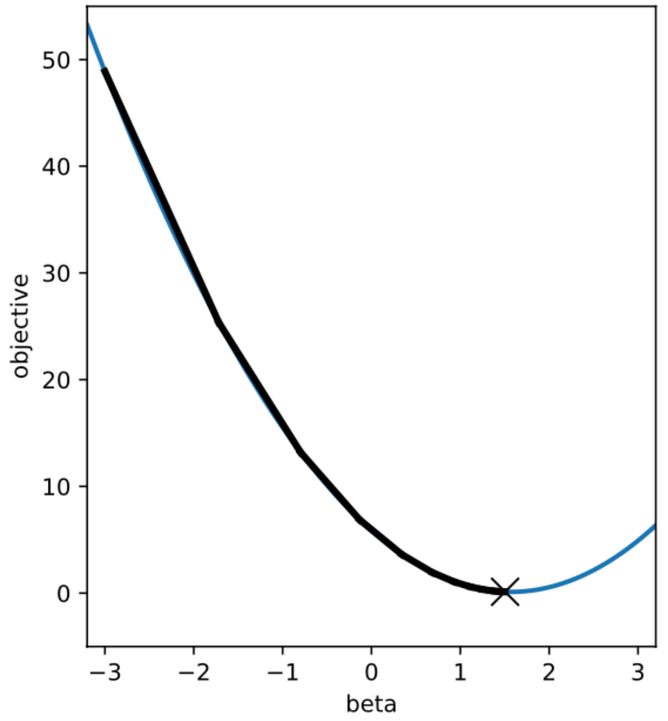

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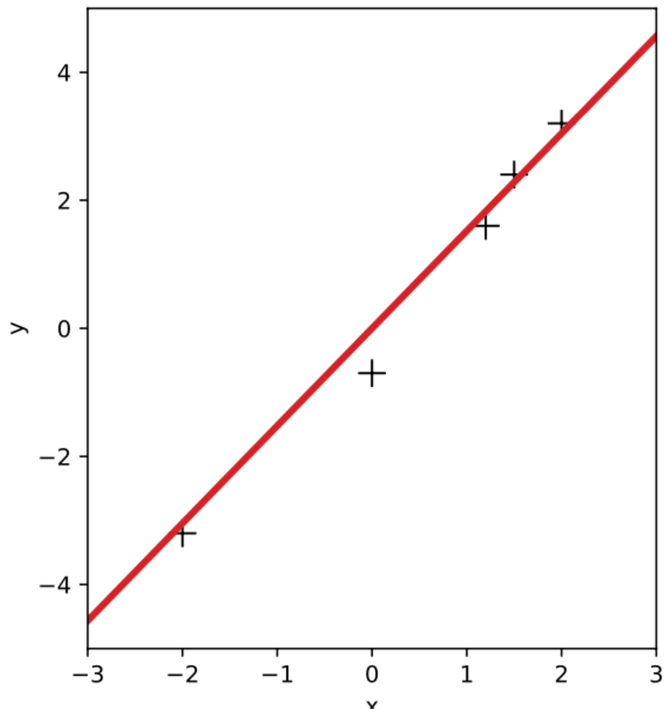

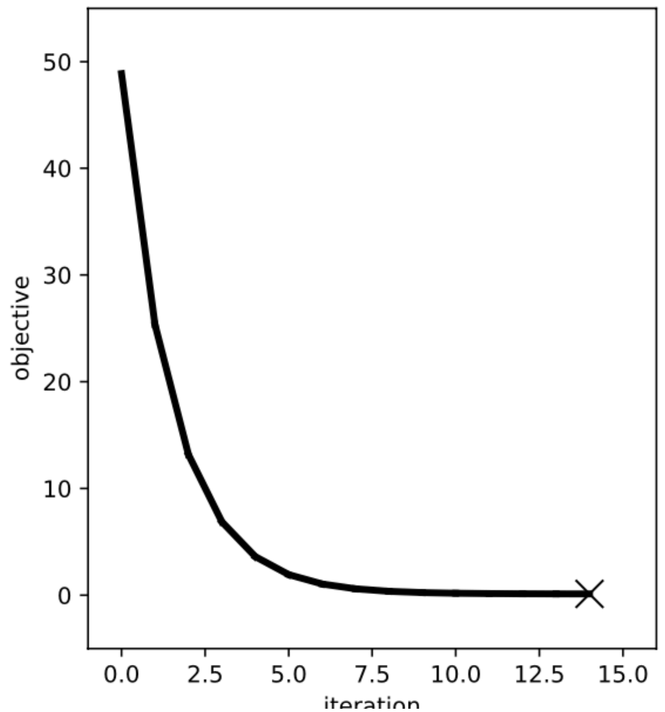

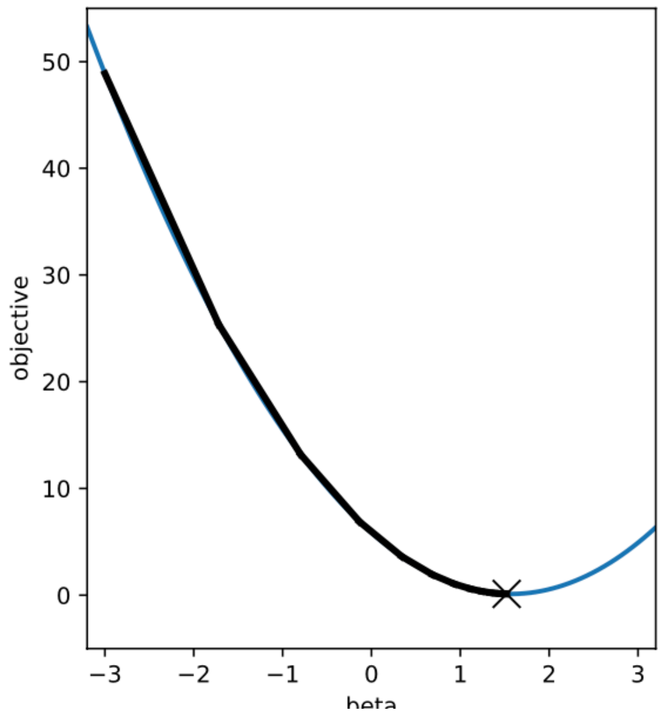

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Goal: estimate the distribution your data come from, aka estimate $p(x)$

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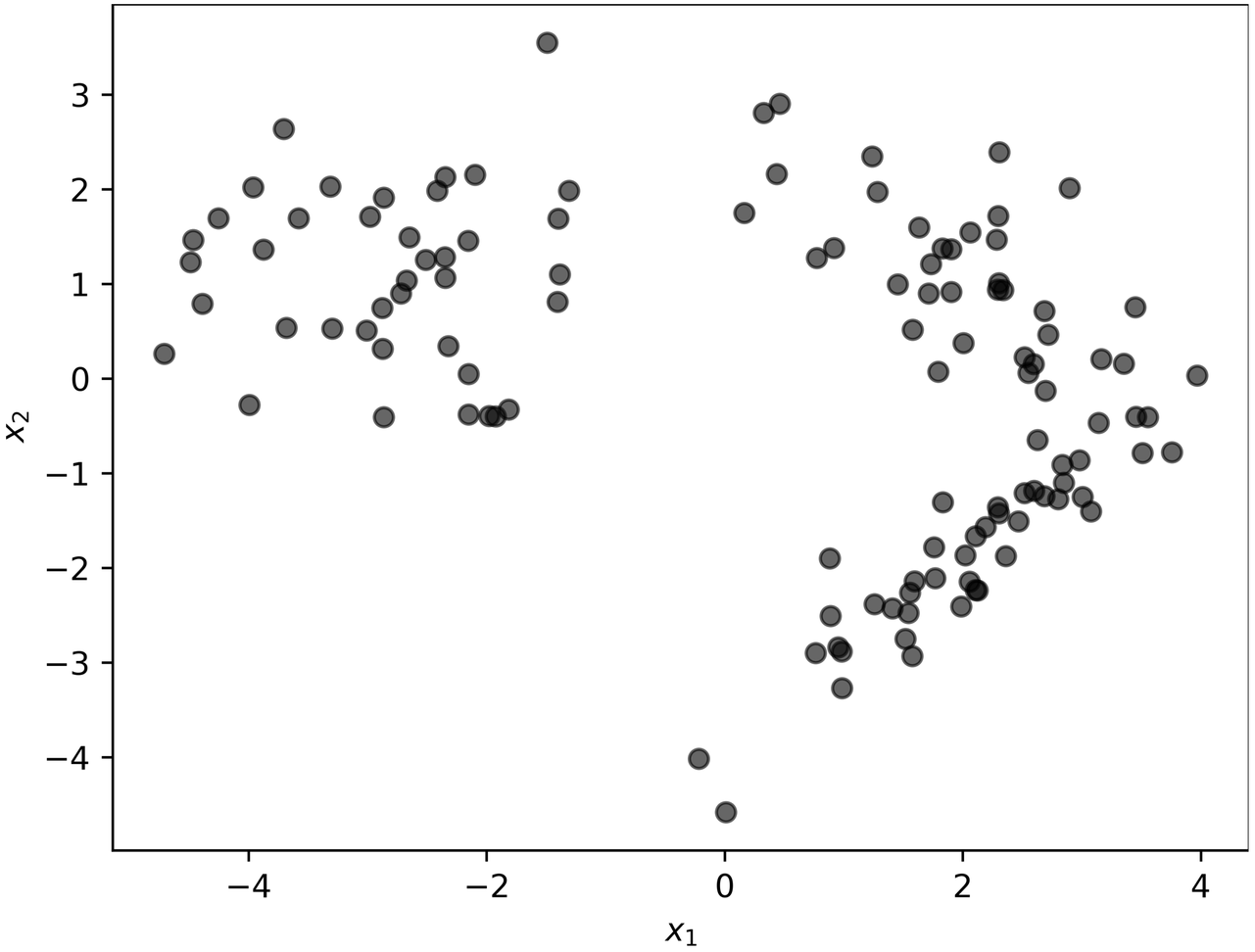

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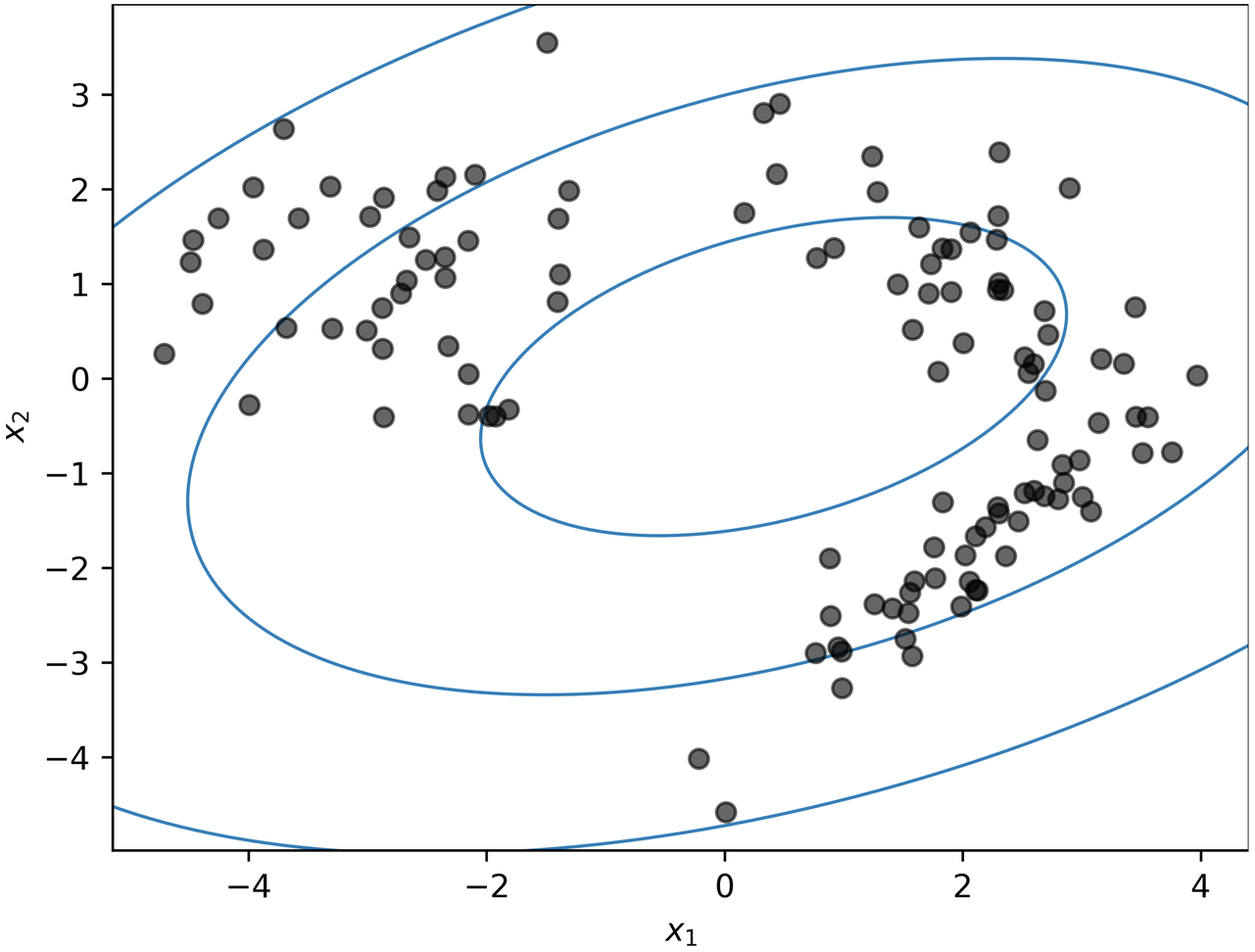

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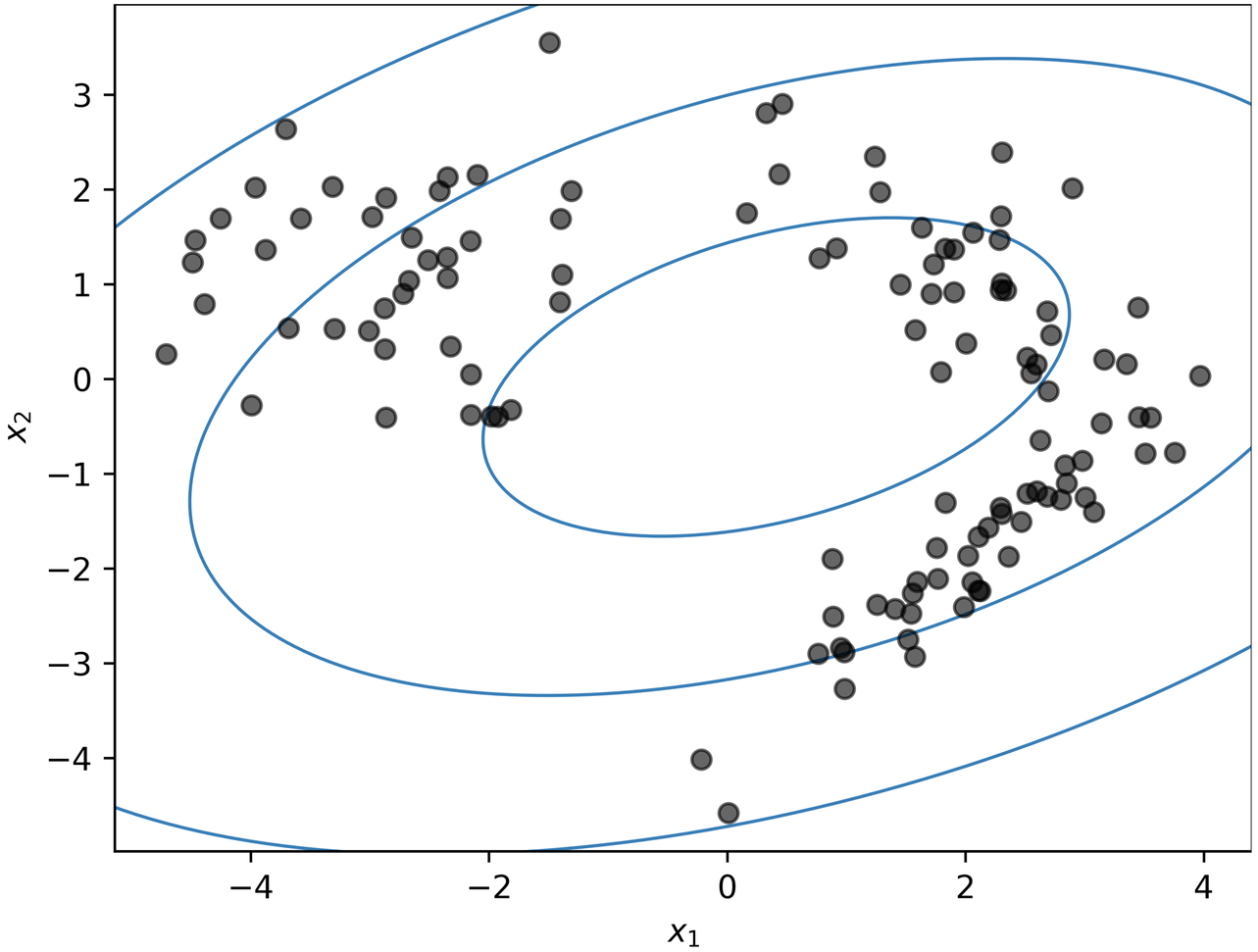

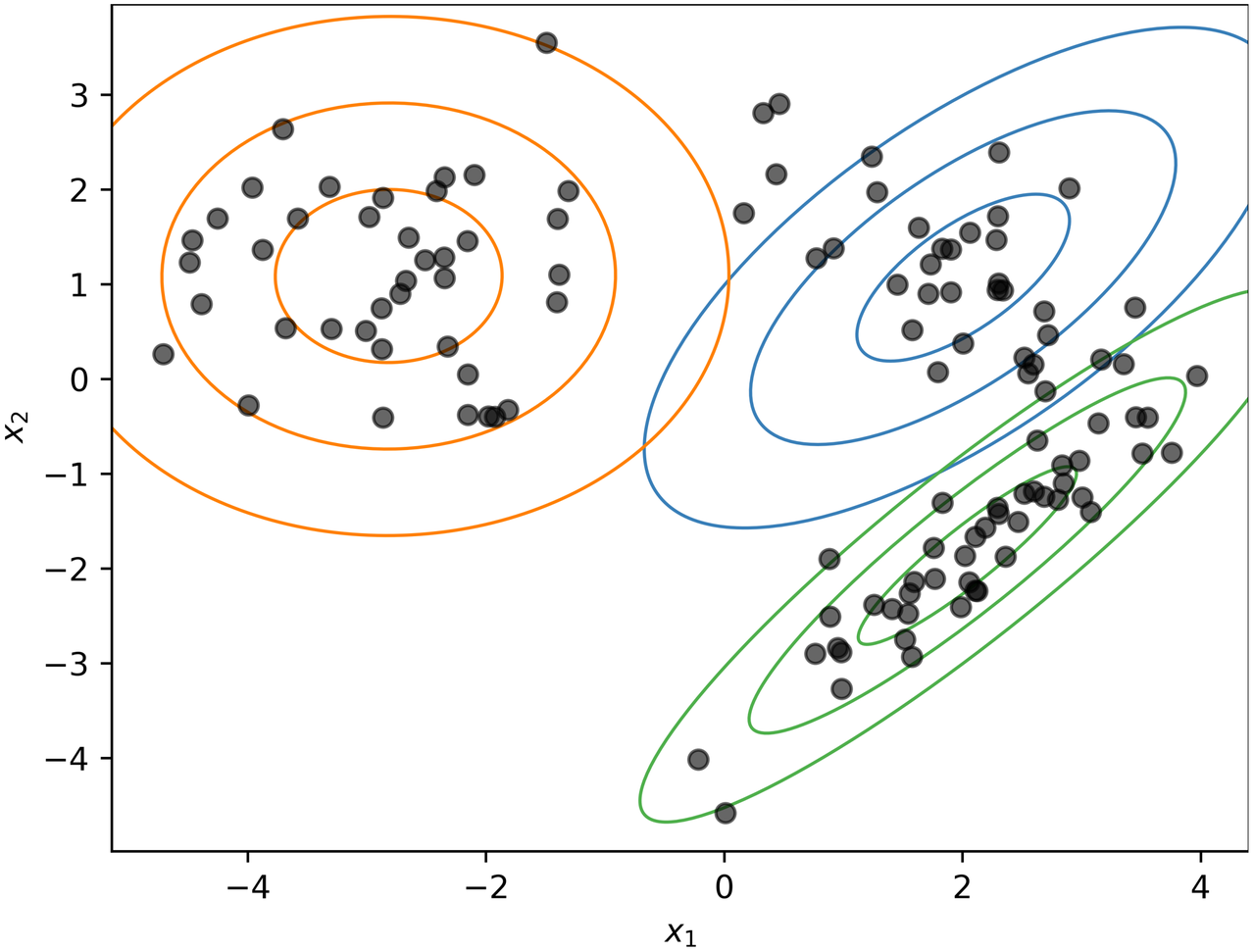

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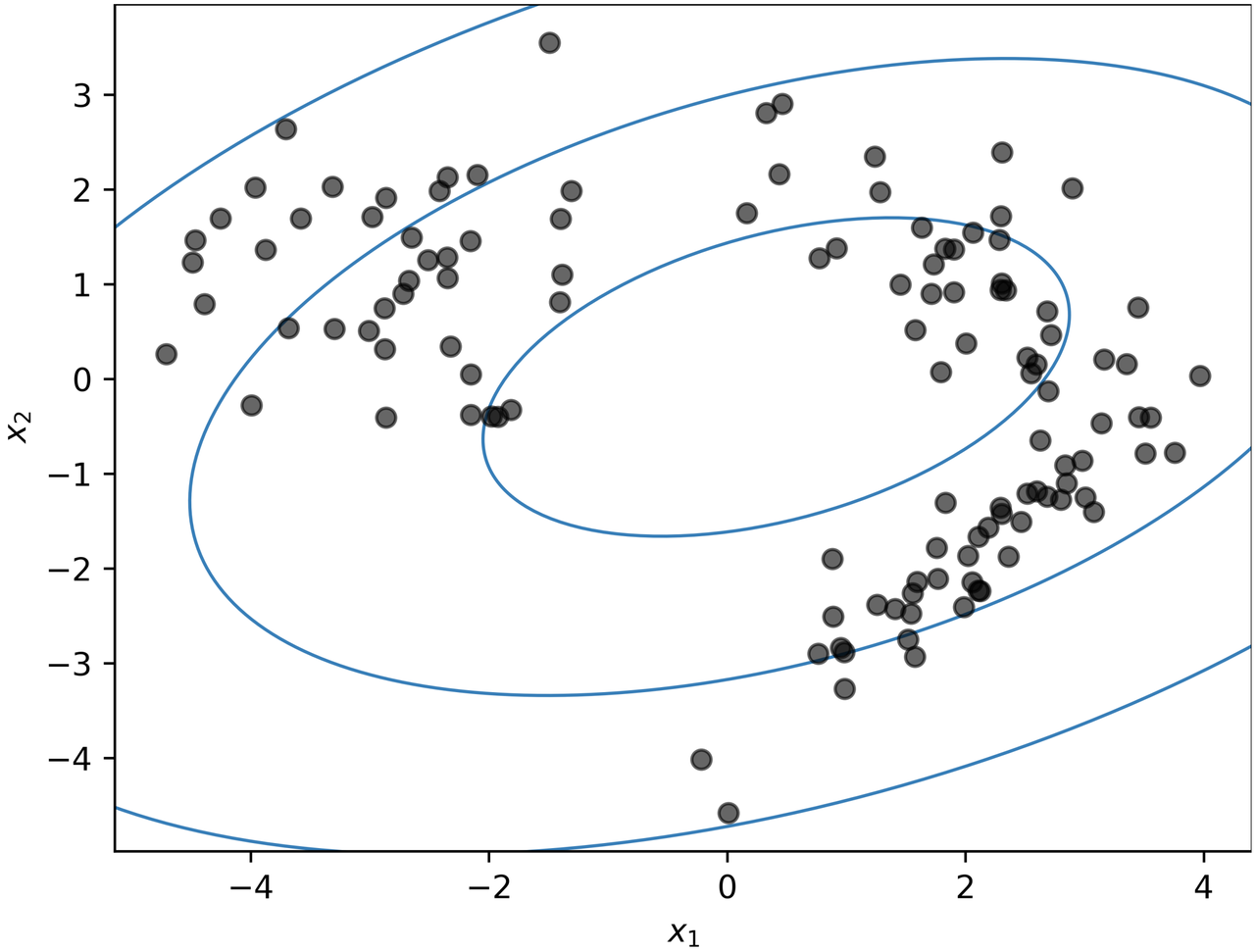

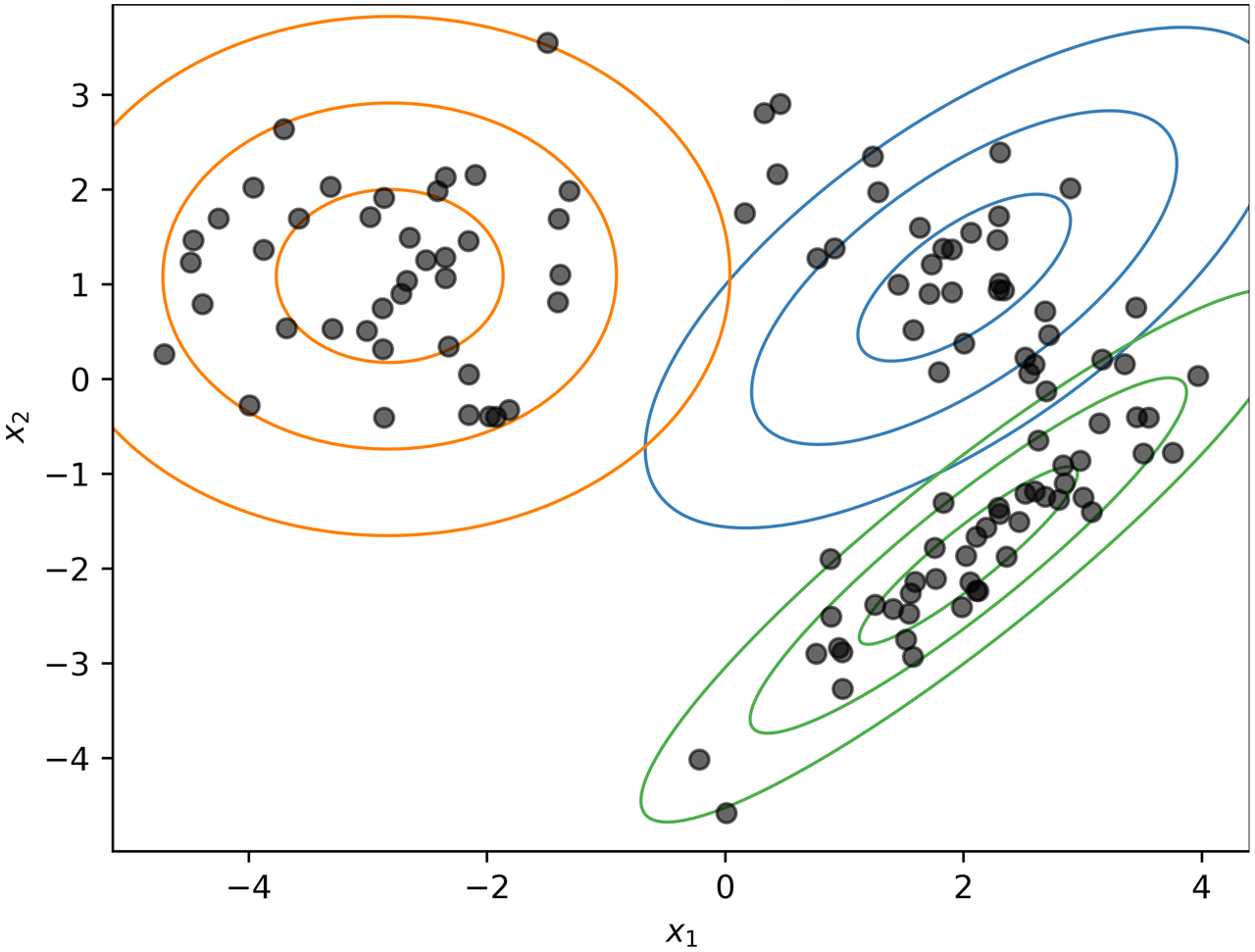

Applications: (1) exploratory analyses, (2) evaluation, (3) synthetic data generation

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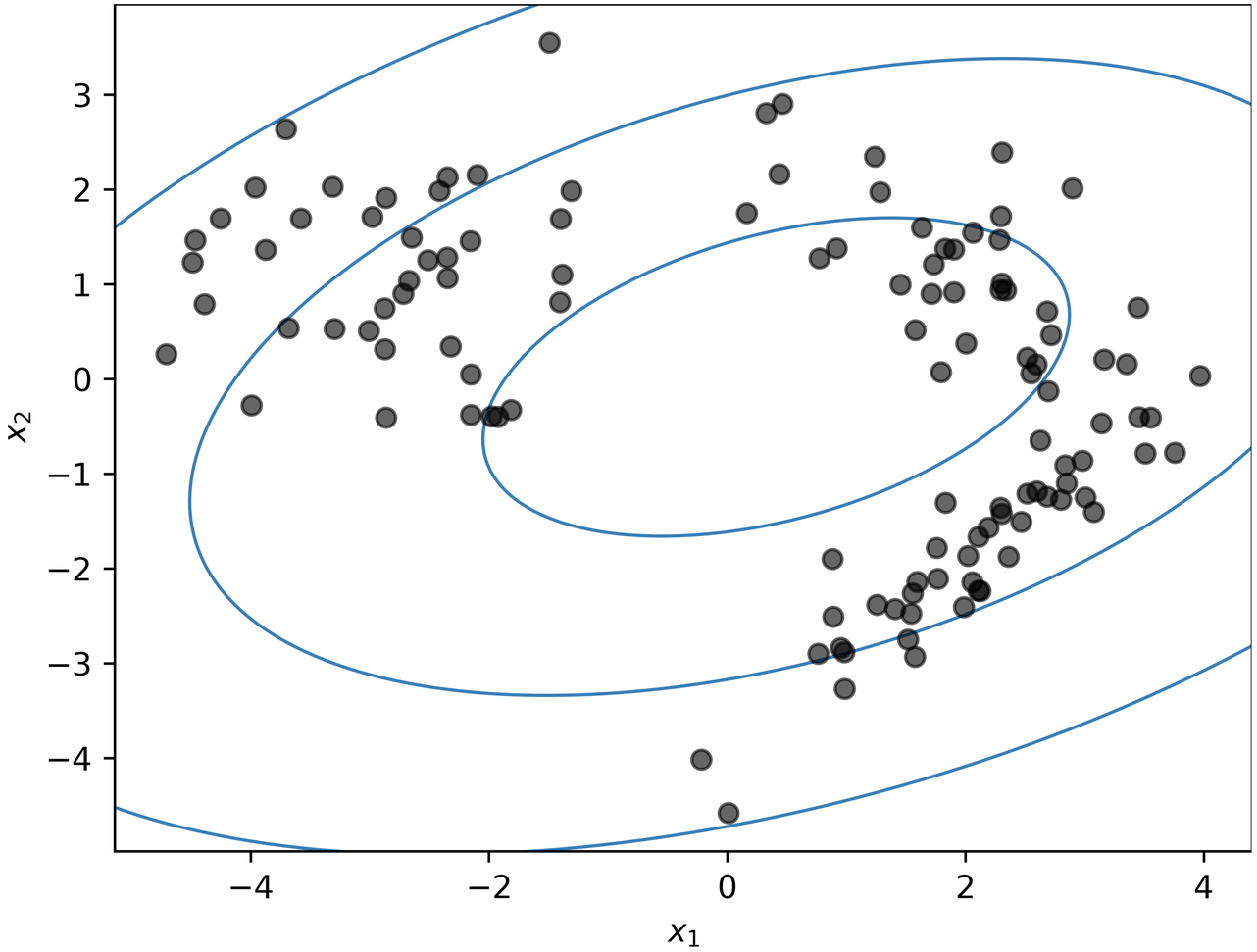

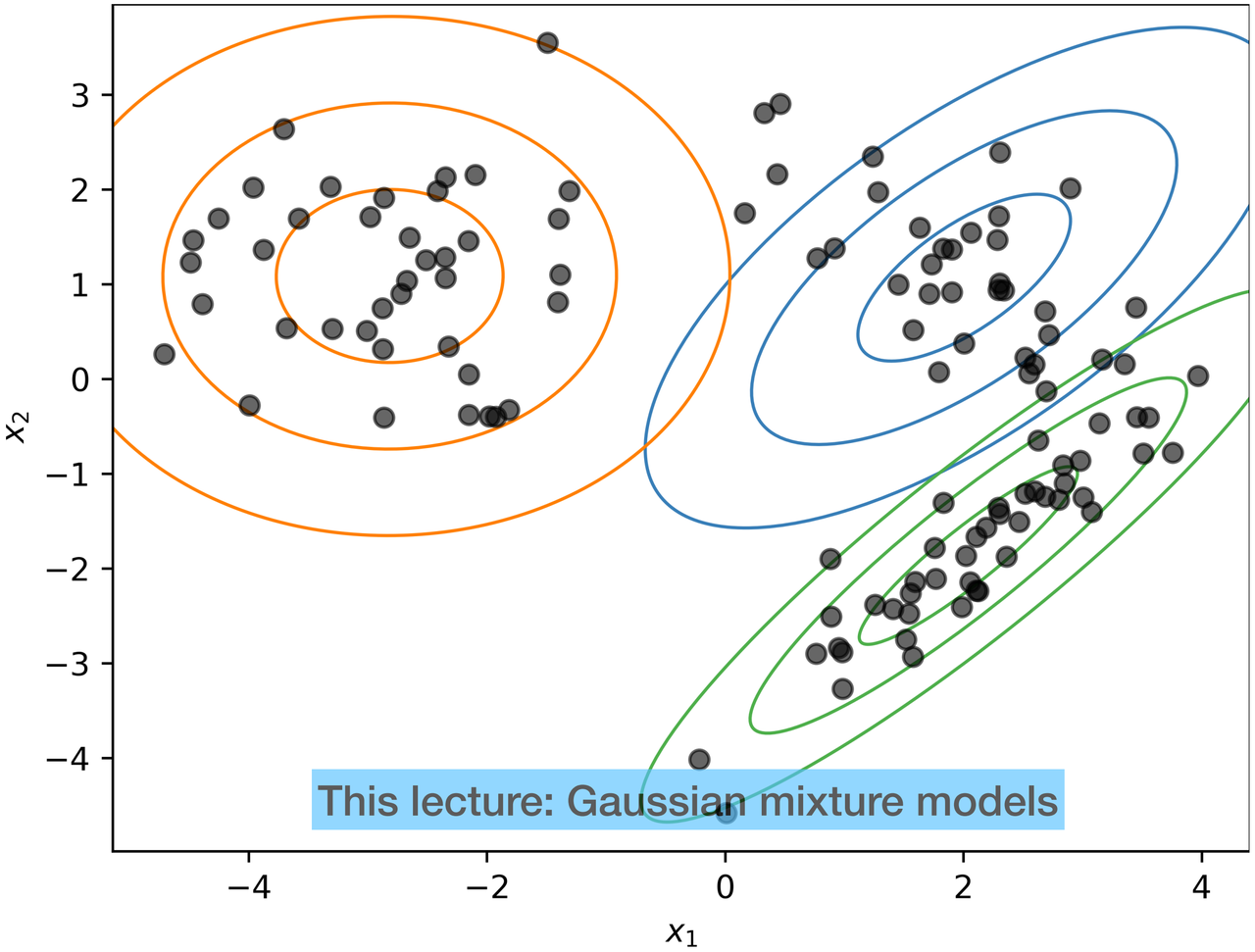

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A D-dimensional multivariate **Gaussian** or **normal** distribution is characterised by a *mean* vector μ and a *covariance matrix* Σ, with

pdf: $p(\mathbf{x} \mid \mu, \Sigma) = (2\pi)^{-\frac{D}{2}} \mid \Sigma \mid^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(\mathbf{x}-\mu)^T \Sigma^{-1}(\mathbf{x}-\mu)\right)$

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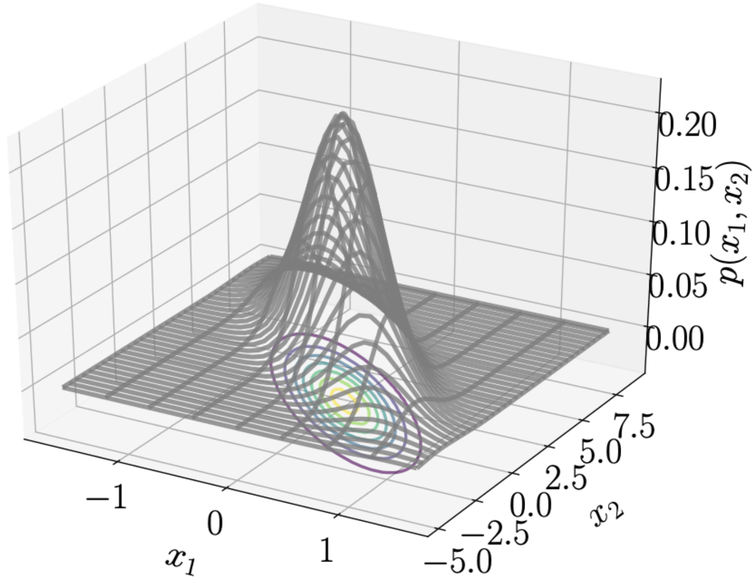

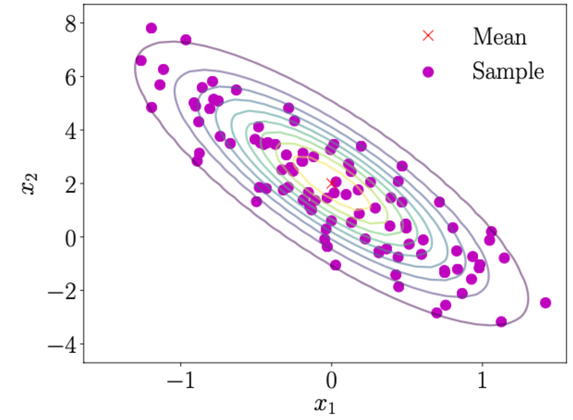

(b) Multivariate (two-dimensional) Gaussian, viewed from top. The red cross shows the mean and the colored lines show the contour lines of the density.

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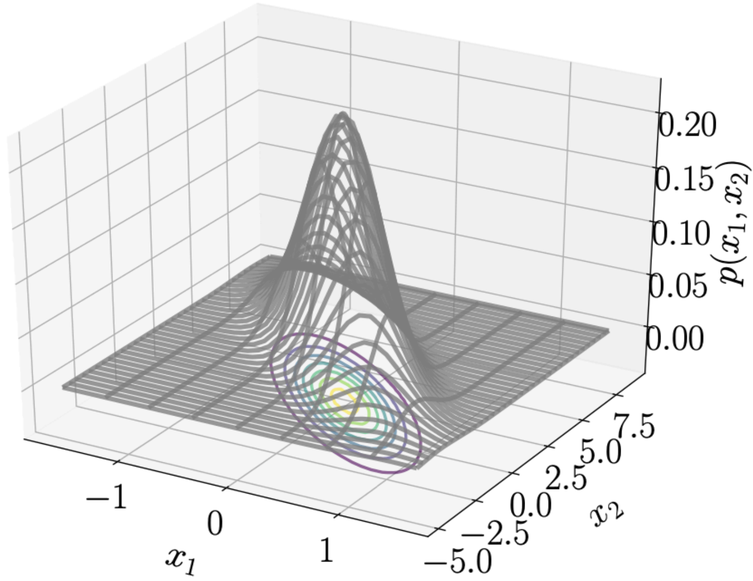

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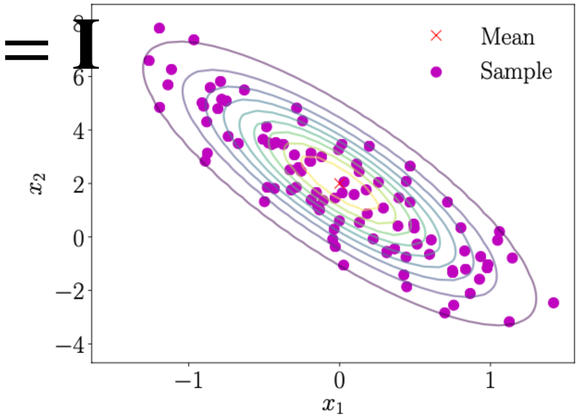
Standard multivariate **Gaussian** or **normal** distribution: $\mu = \mathbf{0}$ and $\Sigma = \mathbf{I}$

When Σ is a diagonal matrix, $p(\mathbf{x}\,|\,\mu,\Sigma) = \prod_{d=1}^{D} p(x_d\,|\,\mu_d,\Sigma_{d,d})$

Diagonal Gaussian, dimensions are independent



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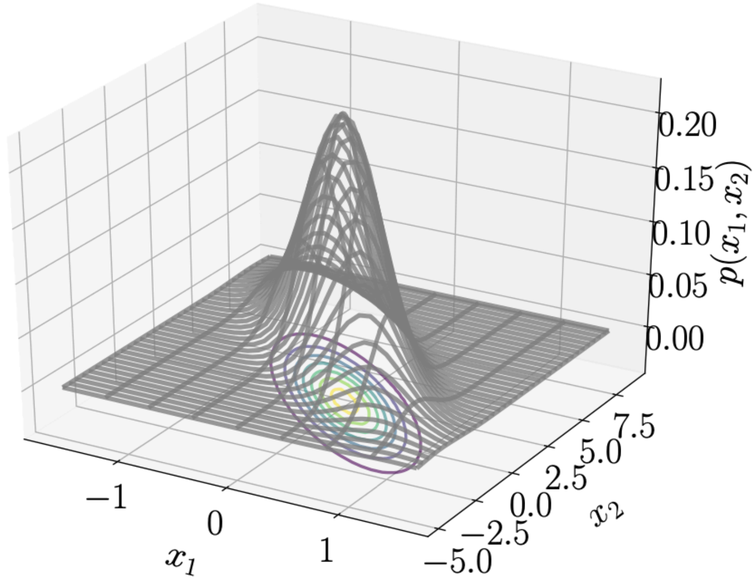

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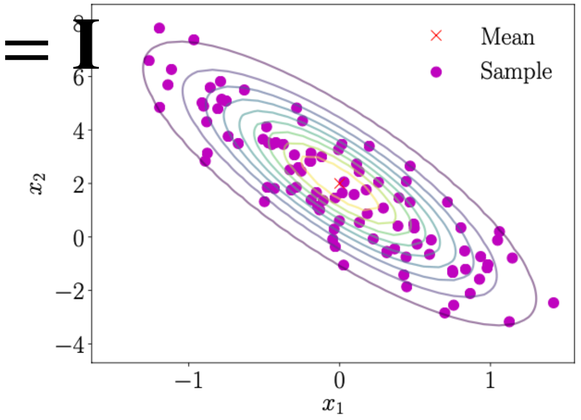
Alternative parameterisation, $\eta_1 = \Sigma^{-1}\mu$ and $\eta_2 = \Sigma^{-1}$ [precision]

Easier for multiplication/division and identifying conditional independence



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The components $p_k(x)$ are, typically, members of a family of basic distributions, e.g., Gaussians, Bernoullis, or Gammas, and π_k's are *mixture weights*.

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When the base distributions are Gaussian distributions $p_k(x) = \mathcal{N}(x; \mu_k, \Sigma_k)$, we have a **Gaussian mixture model (GMM)**:

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$\theta = \{\pi_k, \mu_k, \Sigma_k \text{ for } k = 1,2,\ldots,K\}$ are the parameters of the GMM.

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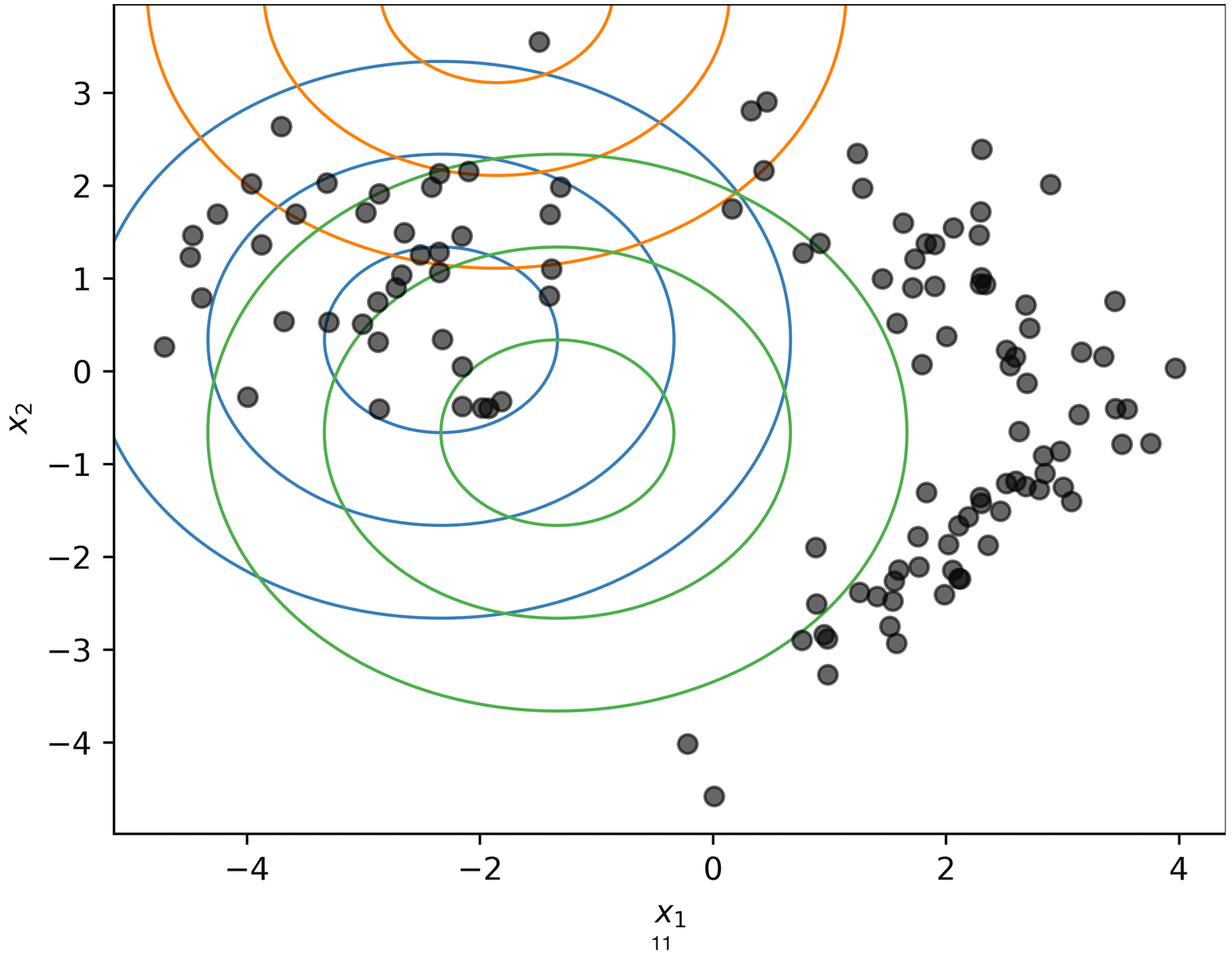

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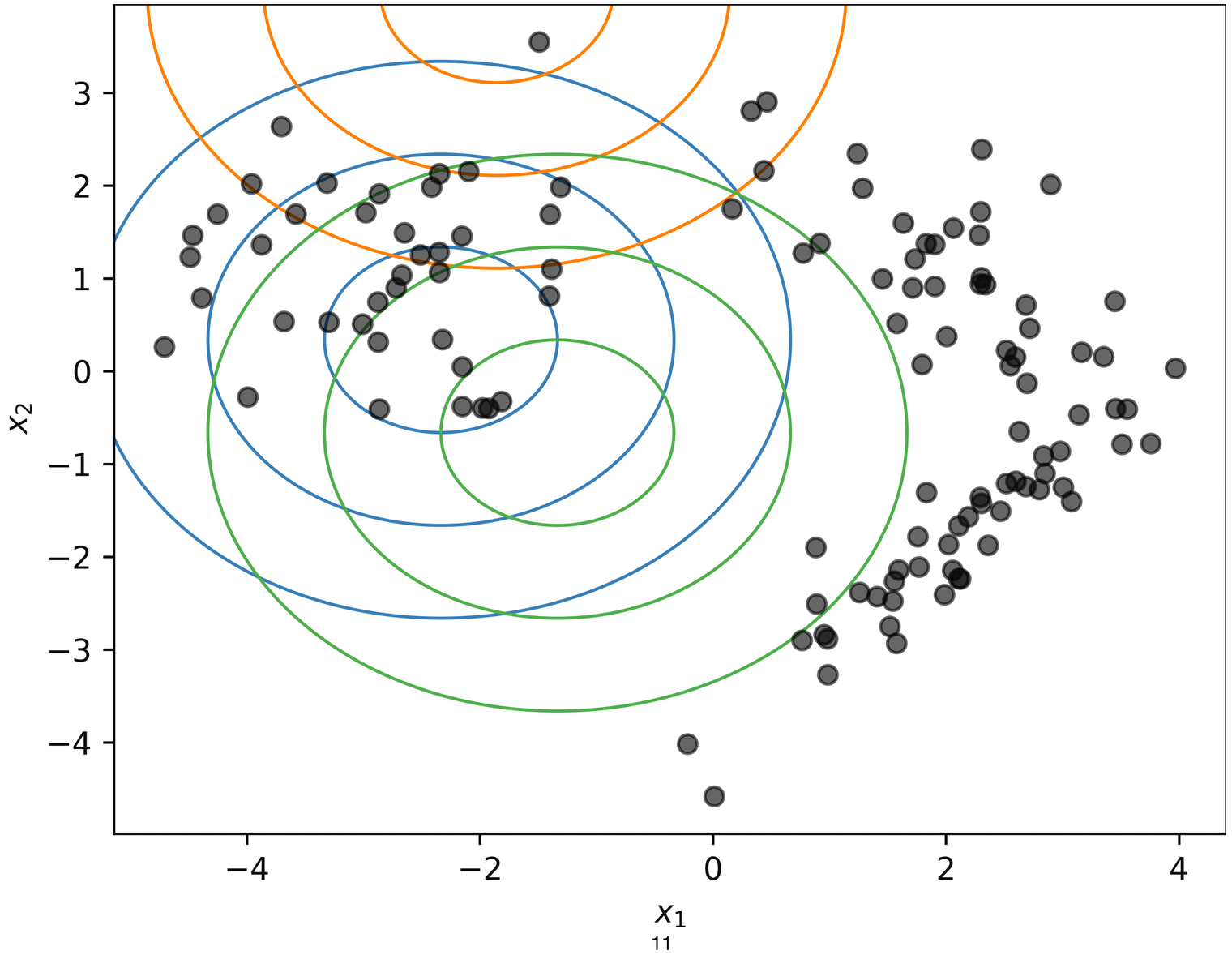

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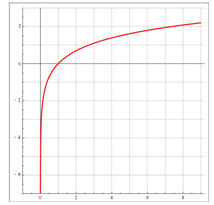

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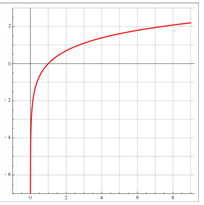

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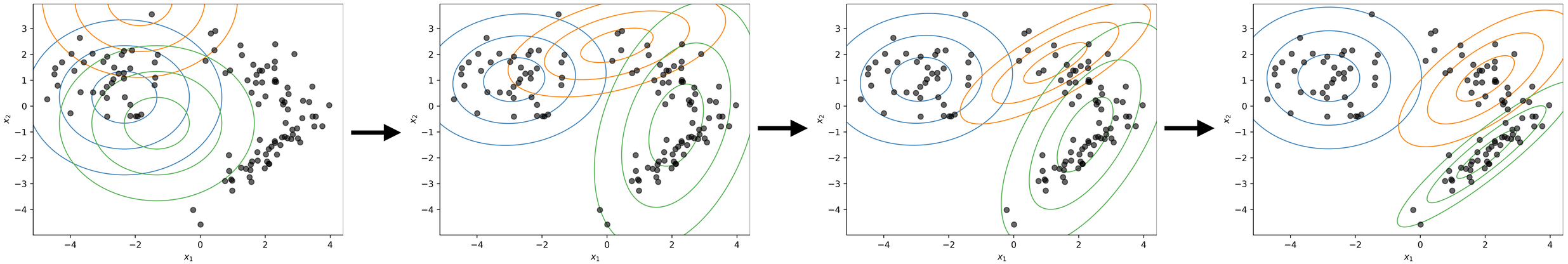
GMMs - log-likelihood gradients

Log-likelihood: $L(\theta) = \log p(X|\theta) = \sum_{n=1}^{N} \log p(x_n|\theta) = \sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k \mathcal{N}(x_n; \mu_k, \Sigma_k)$

Strategy: find the gradients of $L(\theta)$ and try to set them to zero.

$$\frac{\partial}{\partial \mu_k} L = \sum_{n=1}^{N} \frac{\partial \log p(x_n|\theta)}{\partial \mu_k} = \mathbf{0}^\intercal \qquad \frac{\partial}{\partial \Sigma_k} L = \sum_{n=1}^{N} \frac{\partial \log p(x_n|\theta)}{\partial \Sigma_k} = \mathbf{0} \qquad \frac{\partial}{\partial \pi_k} L = \sum_{n=1}^{N} \frac{\partial \log p(x_n|\theta)}{\partial \pi_k} = 0$$

Unlike linear regression, the optimal parameters are not analytically tractable. We resort to an iterative optimisation procedure.



Initialisation *After 50 iterations*

GMMs - iterative procedure

Initialise $\{\pi_k, \mu_k, \Sigma_k\}_{k=1}^K$

Repeat until convergence:

1. **Evaluate responsibilities** r_{nk} for every data point x_n using current parameters:

$$r_{nk} = \frac{\pi_k \mathcal{N}(x_n; \mu_k, \Sigma_k)}{\sum_{j=1}^K \pi_j \mathcal{N}(x_n; \mu_j, \Sigma_j)}$$

2. **Re-estimate parameters** $\{\pi_k, \mu_k, \Sigma_k\}_{k=1}^K$ using the current responsibilities r_{nk}:

$$\mu_k = \frac{1}{N_k} \sum_{n=1}^N r_{nk} x_n, \quad N_k = \sum_{n=1}^N r_{nk}$$

$$\Sigma_k = \frac{1}{N_k} \sum_{n=1}^N r_{nk} (x_n - \mu_k)(x_n - \mu_k)^\intercal$$

$$\pi_k = \frac{N_k}{N}$$

GMMs - responsibility definition

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We define **responsibility** r_{nk} for every data point x_n:

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proportional to the likelihood of the k-th mixture component given the data point x_n

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Note that $\mathbf{r}_n = [r_{n1}, r_{n2}, \ldots, r_{nK}]^\intercal \in \mathbb{R}^D$ is a probability vector, i.e., $\sum_k r_{nk} = 1$ with $r_{nk} \geq 0$

This probability vector distributes probability mass among the K mixture components, and we can think of $\mathbf{r}_n$ as a "soft assignment" of x_n to the K mixture components.

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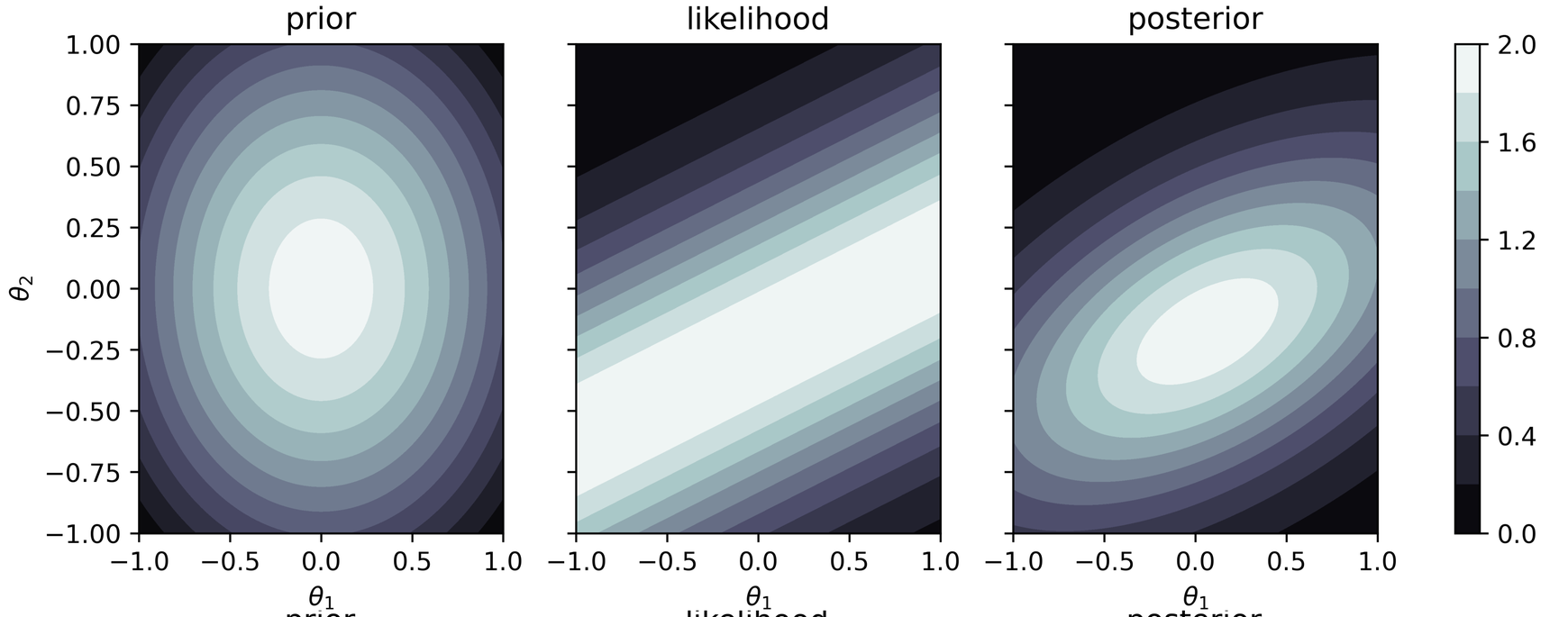
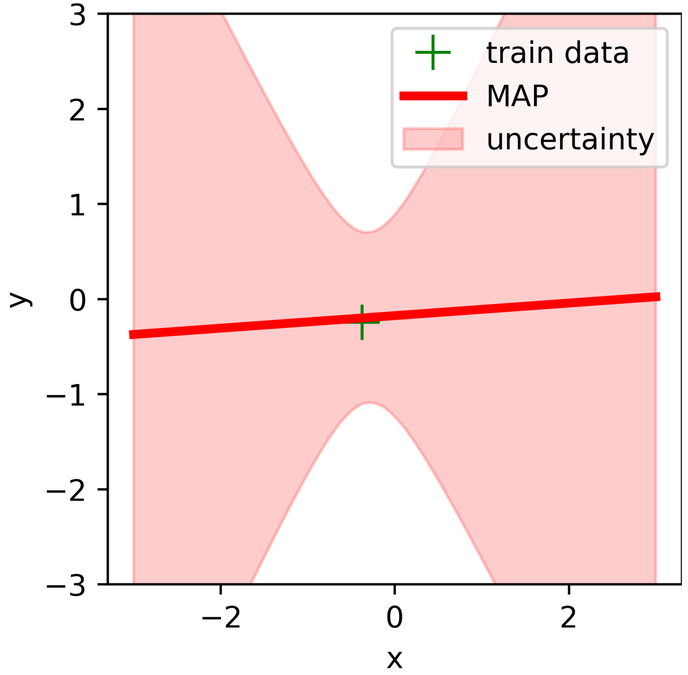
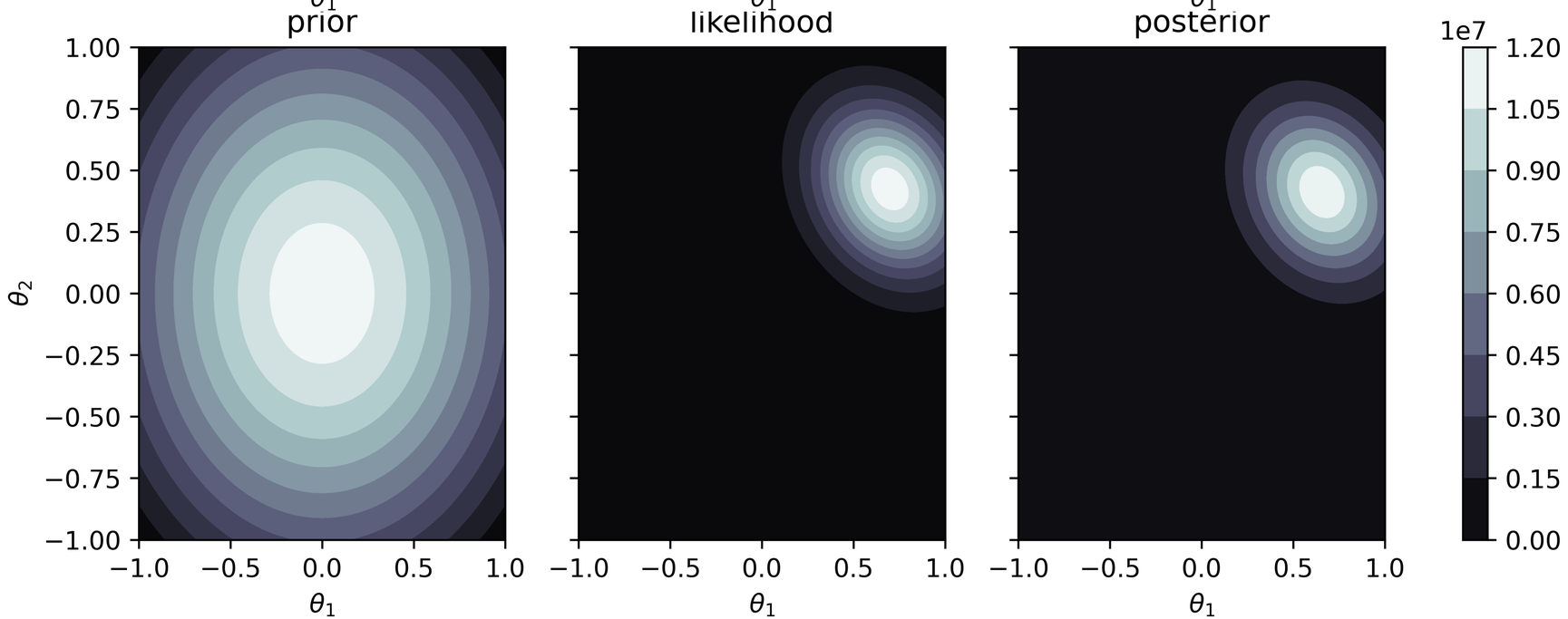
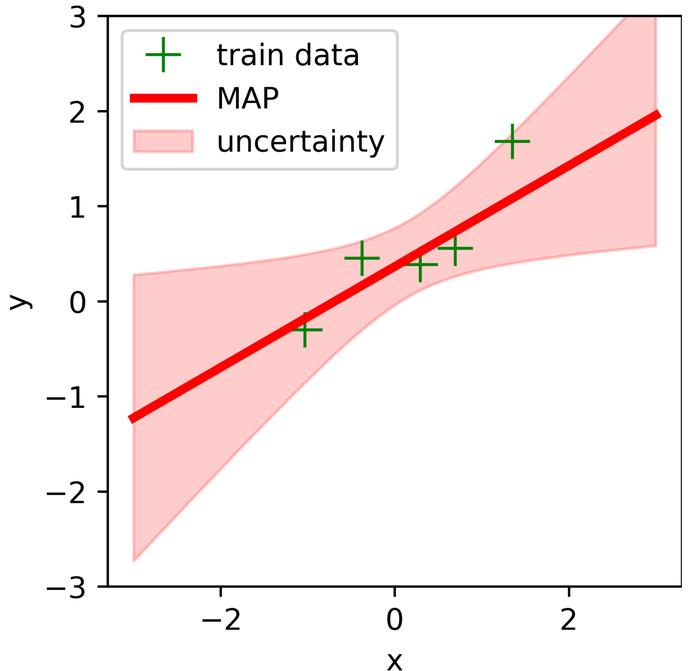
Let's now derive the parameter updates in step 2!

More on Bayesian linear regression









Overview

Last lecture:

1. **Model**: Gaussian mixture models
2. **Learning**: parameter learning using *maximum likelihood*
3. **Iterative** procedure, derive mean update

Initialise $\{\pi_k, \mu_k, \Sigma_k\}_{k=1}^K$

Repeat until convergence:

1. **Evaluate responsibilities** r_{nk} for every data point x_n using current parameters:

$$r_{nk} = \frac{\pi_k \mathcal{N}(x_n; \mu_k, \Sigma_k)}{\sum_{j=1}^K \pi_j \mathcal{N}(x_n; \mu_j, \Sigma_j)}$$

2. **Re-estimate parameters** $\{\pi_k, \mu_k, \Sigma_k\}_{k=1}^K$ using the current responsibilities r_{nk}:

$$\mu_k = \frac{1}{N_k} \sum_{n=1}^N r_{nk} x_n, \quad N_k = \sum_{n=1}^N r_{nk}$$

$$\Sigma_k = \frac{1}{N_k} \sum_{n=1}^N r_{nk} (x_n - \mu_k)(x_n - \mu_k)^\intercal$$

$$\pi_k = \frac{N_k}{N}$$

This lecture:

1. Derive covariance and mixture weight updates
2. Issues with maximum likelihood and workarounds
3. K-means as a special case
4. Theoretical foundation: EM algorithm (1 is E step, 2 is M step)

Recap: Gaussian mixture models and how to find θ

Model: $$p_\theta(x) = \sum_{k=1}^{K} \pi_k \mathcal{N}(x; \mu_k, \Sigma_k) \qquad 0 \leq \pi_k \leq 1, \sum_{k=1}^{K} \pi_k = 1$$

where we defined $\theta = \{\pi_k, \mu_k, \Sigma_k \text{ for } k = 1,2,\ldots,K\}$ as the parameters of the GMM.

Data: $\mathbf{X} = \{x_1, x_2, \ldots, x_N\}$, where x_n's are drawn i.i.d. from an unknown distribution $p(x)$.

Objective: find a *good* approximation/representation of this unknown density $p(x)$ by means of a GMM with K components, that is finding θ.

$$P(\theta \mid \mathcal{D}) = \frac{P(\theta, \mathcal{D})}{P(\mathcal{D})} = \frac{P(\theta)\, P(\mathcal{D} \mid \theta)}{P(\mathcal{D})}$$

Weeks 6 and 7

This week

- Maximum likelihood (ML/MLE), $\text{argmax}_\theta\ p(\mathcal{D} \mid \theta)$
- Maximum a-posteriori (MAP), $\text{argmax}_\theta\ p(\mathcal{D} \mid \theta)p(\theta)$
- Exact/approximate Bayesian inference

Recap: GMMs - iterative procedure

Initialise $\{\pi_k, \mu_k, \Sigma_k\}_{k=1}^K$

Repeat until convergence:

1. **Evaluate responsibilities** r_{nk} for every data point x_n using current parameters:

$$r_{nk} = \frac{\pi_k \mathcal{N}(x_n; \mu_k, \Sigma_k)}{\sum_{j=1}^K \pi_j \mathcal{N}(x_n; \mu_j, \Sigma_j)}$$

2. **Re-estimate parameters** $\{\pi_k, \mu_k, \Sigma_k\}_{k=1}^K$ using the current responsibilities r_{nk}:

$$\mu_k = \frac{1}{N_k} \sum_{n=1}^N r_{nk} x_n, \quad N_k = \sum_{n=1}^N r_{nk}$$

$$\Sigma_k = \frac{1}{N_k} \sum_{n=1}^N r_{nk} (x_n - \mu_k)(x_n - \mu_k)^\intercal$$

$$\pi_k = \frac{N_k}{N}$$

Recap: Step 2, mean update

$$L(\theta) = \sum_{n} \log p(x_n \mid \theta) = \sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k \mathcal{N}(x_n; \mu_k, \Sigma_k)$$

Log likelihood

Recap: Step 2, mean update

$$L(\theta) = \sum_n \log p(x_n \mid \theta) = \sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k \mathcal{N}(x_n; \mu_k, \Sigma_k)$$

Log likelihood

$$\frac{\partial L(\theta)}{\partial \mu_k} = \sum_{n=1}^{N} \frac{1}{p(x_n \mid \theta)} \frac{\partial}{\partial \mu_k} \sum_{j=1}^{K} \pi_j \mathcal{N}(x_n; \mu_j, \Sigma_j)$$

gradient of log likelihood wrt mean

Recap: Step 2, mean update

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Ignore terms that do not depend on k

Recap: Step 2, mean update

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$$= \sum_{n=1}^{N} \frac{1}{p(x_n \mid \theta)} \pi_k \mathcal{N}(x_n; \mu_k, \Sigma_k) \left(x_n - \mu_k\right)^\intercal \Sigma_k^{-1}$$

Gradient of Gaussian wrt mean

Recap: Step 2, mean update

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Gradient of Gaussian wrt mean

$$= \sum_{n=1}^{N} r_{nk} \left(x_n - \mu_k\right)^\intercal \Sigma_k^{-1}$$

Rewrite using responsibility

Recap: Step 2, mean update

$$L(\theta) = \sum_n \log p(x_n \mid \theta) = \sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k \mathcal{N}(x_n; \mu_k, \Sigma_k)$$

Log likelihood

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Gradient of Gaussian wrt mean

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Rewrite using responsibility

$$\frac{\partial L(\theta)}{\partial \mu_k} = \mathbf{0}^\intercal \rightarrow \mu_k = \frac{\sum_n r_{nk} x_n}{\sum_n r_{nk}}$$

Set gradient to zero

Step 2, covariance update [1]

$$L(\theta) = \sum_{n} \log p(x_n \mid \theta) = \sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k \mathcal{N}(x_n; \mu_k, \Sigma_k)$$

Log likelihood

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Log likelihood

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gradient of log likelihood wrt cov

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Log likelihood

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Ignore terms that do not depend on k

$$\frac{\partial}{\partial \Sigma_k} \mathcal{N}(x_n; \mu_k, \Sigma_k) = \frac{\partial}{\partial \Sigma_k} \left[(2\pi)^{-\frac{D}{2}} \mid \Sigma_k \mid^{-\frac{1}{2}} \exp\left(-\frac{1}{2} (x_n - \mu_k)^T \Sigma_k^{-1} (x_n - \mu_k) \right) \right]$$

Gradient of Gaussian wrt cov

Step 2, covariance update [1]

$$L(\theta) = \sum_n \log p(x_n \mid \theta) = \sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k \mathcal{N}(x_n; \mu_k, \Sigma_k)$$

Log likelihood

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Gradient of Gaussian wrt cov

$$= (2\pi)^{-\frac{D}{2}} \frac{-1}{2} \mid \Sigma_k \mid^{-\frac{1}{2}} \Sigma_k^{-1} \exp\left(-\frac{1}{2} (x_n - \mu_k)^T \Sigma_k^{-1} (x_n - \mu_k) \right)$$

$$+ (2\pi)^{-\frac{D}{2}} \mid \Sigma_k \mid^{-\frac{1}{2}} \exp\left(-\frac{1}{2} (x_n - \mu_k)^T \Sigma_k^{-1} (x_n - \mu_k) \right) \frac{1}{2} \Sigma_k^{-1} (x_n - \mu_k)(x_n - \mu_k)^\intercal \Sigma_k^{-1}$$

Step 2, covariance update [1]

$$L(\theta) = \sum_n \log p(x_n \mid \theta) = \sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k \mathcal{N}(x_n; \mu_k, \Sigma_k)$$

Log likelihood

$$\frac{\partial L(\theta)}{\partial \Sigma_k} = \sum_{n=1}^{N} \frac{1}{p(x_n \mid \theta)} \frac{\partial}{\partial \Sigma_k} \sum_{j=1}^{K} \pi_j \mathcal{N}(x_n; \mu_j, \Sigma_j)$$

gradient of log likelihood wrt cov

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Ignore terms that do not depend on k

$$\frac{\partial}{\partial \Sigma_k} \mathcal{N}(x_n; \mu_k, \Sigma_k) = \frac{\partial}{\partial \Sigma_k} \left[(2\pi)^{-\frac{D}{2}} |\Sigma_k|^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(x_n - \mu_k)^T \Sigma_k^{-1} (x_n - \mu_k) \right) \right]$$

Gradient of Gaussian wrt cov

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$$= -\frac{1}{2} \mathcal{N}(x_n; \mu_k, \Sigma_k) [\Sigma_k^{-1} - \Sigma_k^{-1} (x_n - \mu_k)(x_n - \mu_k)^\intercal \Sigma_k^{-1}]$$

Step 2, covariance update [2]

gradient of log likelihood wrt cov

$$\frac{\partial L(\theta)}{\partial \Sigma_k} = \sum_{n=1}^{N} \frac{1}{p(x_n \mid \theta)} \pi_k \frac{-1}{2} \mathcal{N}(x_n; \mu_k, \Sigma_k)[\Sigma_k^{-1} - \Sigma_k^{-1}(x_n - \mu_k)(x_n - \mu_k)^\intercal \Sigma_k^{-1}]$$

Step 2, covariance update [2]

gradient of log likelihood wrt cov

$$\frac{\partial L(\theta)}{\partial \Sigma_k} = \sum_{n=1}^{N} \frac{1}{p(x_n \mid \theta)} \pi_k \frac{-1}{2} \mathcal{N}(x_n; \mu_k, \Sigma_k)[\Sigma_k^{-1} - \Sigma_k^{-1}(x_n - \mu_k)(x_n - \mu_k)^\intercal \Sigma_k^{-1}]$$

$$= -\frac{1}{2} \sum_{n=1}^{N} r_{nk}[\Sigma_k^{-1} - \Sigma_k^{-1}(x_n - \mu_k)(x_n - \mu_k)^\intercal \Sigma_k^{-1}]$$

Rewrite using responsibility

Step 2, covariance update [2]

gradient of log likelihood wrt cov

$$\frac{\partial L(\theta)}{\partial \Sigma_k} = \sum_{n=1}^{N} \frac{1}{p(x_n \mid \theta)} \pi_k \frac{-1}{2} \mathcal{N}(x_n; \mu_k, \Sigma_k)[\Sigma_k^{-1} - \Sigma_k^{-1}(x_n - \mu_k)(x_n - \mu_k)^\intercal \Sigma_k^{-1}]$$

Rewrite using responsibility

$$= -\frac{1}{2} \sum_{n=1}^{N} r_{nk}[\Sigma_k^{-1} - \Sigma_k^{-1}(x_n - \mu_k)(x_n - \mu_k)^\intercal \Sigma_k^{-1}]$$

Set gradient to zero

$$\frac{\partial L(\theta)}{\partial \Sigma_k} = \mathbf{0} \rightarrow \Sigma_k = \frac{\sum_n r_{nk}(x_n - \mu_k)(x_n - \mu_k)^\intercal}{\sum_n r_{nk}}$$

Step 2, covariance update [2]

gradient of log likelihood wrt cov

$$\frac{\partial L(\theta)}{\partial \Sigma_k} = \sum_{n=1}^{N} \frac{1}{p(x_n \mid \theta)} \pi_k \frac{-1}{2} \mathcal{N}(x_n; \mu_k, \Sigma_k)[\Sigma_k^{-1} - \Sigma_k^{-1}(x_n - \mu_k)(x_n - \mu_k)^\intercal \Sigma_k^{-1}]$$

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Set gradient to zero

$$\frac{\partial L(\theta)}{\partial \Sigma_k} = \mathbf{0} \rightarrow \Sigma_k = \frac{\sum_n r_{nk}(x_n - \mu_k)(x_n - \mu_k)^\intercal}{\sum_n r_{nk}}$$

New covariance = weighted covariance of data where weights = responsibilities

Step 2, mixture weight update

$$L(\theta) = \sum_{n} \log p(x_n \mid \theta) = \sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k \mathcal{N}(x_n; \mu_k, \Sigma_k)$$

Log likelihood

Step 2, mixture weight update

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Log likelihood

$$\hat{L}(\theta) = \sum_n \log p(x_n \mid \theta) = \sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k \mathcal{N}(x_n; \mu_k, \Sigma_k) + \lambda \left(\sum_{k=1}^{K} \pi_k - 1 \right)$$

Lagrangian to deal with equality constraint $\sum_k \pi_k = 1$

Covered in optimisation and advanced ML

Step 2, mixture weight update

$$L(\theta) = \sum_n \log p(x_n \mid \theta) = \sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k \mathcal{N}(x_n; \mu_k, \Sigma_k)$$

Log likelihood

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Lagrangian to deal with equality constraint $\sum_k \pi_k = 1$

Covered in optimisation and advanced ML

$$\frac{\partial \hat{L}(\theta)}{\partial \pi_k} = \sum_{n=1}^{N} \frac{1}{p(x_n \mid \theta)} \frac{\partial}{\partial \pi_k} \sum_{j=1}^{K} \pi_j \mathcal{N}(x_n; \mu_j, \Sigma_j) + \frac{\partial}{\partial \pi_k} \lambda \left(\sum_{k=1}^{K} \pi_k - 1 \right)$$

gradient of Lagrangian wrt cov

Step 2, mixture weight update

$$L(\theta) = \sum_n \log p(x_n \mid \theta) = \sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k \mathcal{N}(x_n; \mu_k, \Sigma_k)$$

Log likelihood

$$\hat{L}(\theta) = \sum_n \log p(x_n \mid \theta) = \sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k \mathcal{N}(x_n; \mu_k, \Sigma_k) + \lambda \left(\sum_{k=1}^{K} \pi_k - 1 \right)$$

Lagrangian to deal with equality constraint $\sum_k \pi_k = 1$

Covered in optimisation and advanced ML

$$\frac{\partial \hat{L}(\theta)}{\partial \pi_k} = \sum_{n=1}^{N} \frac{1}{p(x_n \mid \theta)} \frac{\partial}{\partial \pi_k} \sum_{j=1}^{K} \pi_j \mathcal{N}(x_n; \mu_j, \Sigma_j) + \frac{\partial}{\partial \pi_k} \lambda \left(\sum_{k=1}^{K} \pi_k - 1 \right)$$

gradient of Lagrangian wrt cov

$$= \sum_{n=1}^{N} \frac{1}{p(x_n \mid \theta)} \mathcal{N}(x_n; \mu_k, \Sigma_k) \quad + \quad \lambda$$

Ignore terms that do not depend on k

Step 2, mixture weight update

$$L(\theta) = \sum_n \log p(x_n \mid \theta) = \sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k \mathcal{N}(x_n; \mu_k, \Sigma_k)$$

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Ignore terms that do not depend on k

$$= \sum_{n=1}^{N} \frac{r_{nk}}{\pi_k} \quad + \quad \lambda$$

Rewrite using responsibility

Step 2, mixture weight update

$$L(\theta) = \sum_n \log p(x_n \mid \theta) = \sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k \mathcal{N}(x_n; \mu_k, \Sigma_k)$$

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Rewrite using responsibility

$$\frac{\partial \hat{L}(\theta)}{\partial \lambda} = \sum_{k=1}^{K} \pi_k - 1$$

gradient wrt Lagrange multiplier

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$$= \sum_{n=1}^{N} \frac{r_{nk}}{\pi_k} \quad + \quad \lambda$$

Rewrite using responsibility

$$\frac{\partial \hat{L}(\theta)}{\partial \lambda} = \sum_{k=1}^{K} \pi_k - 1$$

gradient wrt Lagrange multiplier

$$\frac{\partial \hat{L}(\theta)}{\partial \pi_k} = 0 \quad \text{and} \quad \frac{\partial \hat{L}(\theta)}{\partial \lambda} = 0 \rightarrow \pi_k = \frac{\sum_n r_{nk}}{N}$$

Set gradients to zero

Overview

Last lecture:

1. **Model**: Gaussian mixture models
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Initialise $\{\pi_k, \mu_k, \Sigma_k\}_{k=1}^K$

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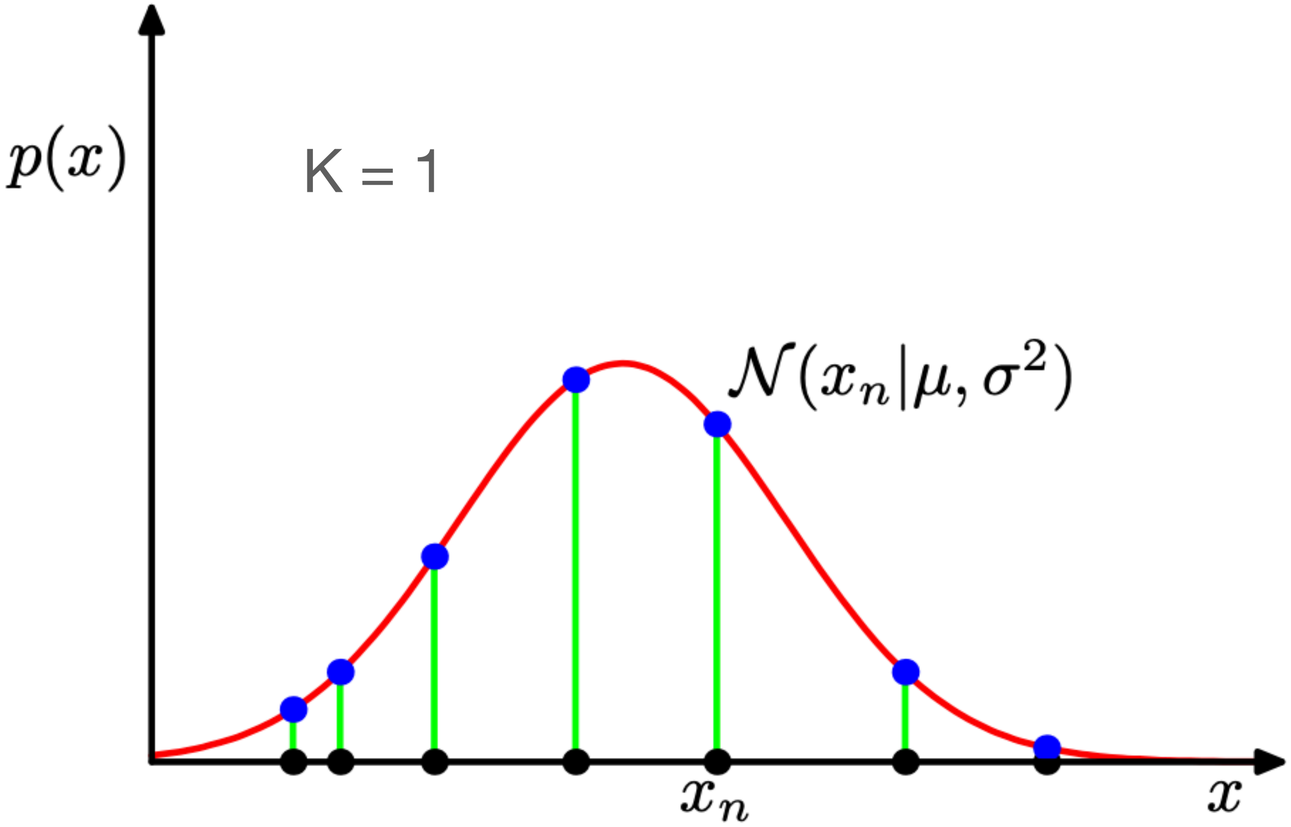
This lecture:

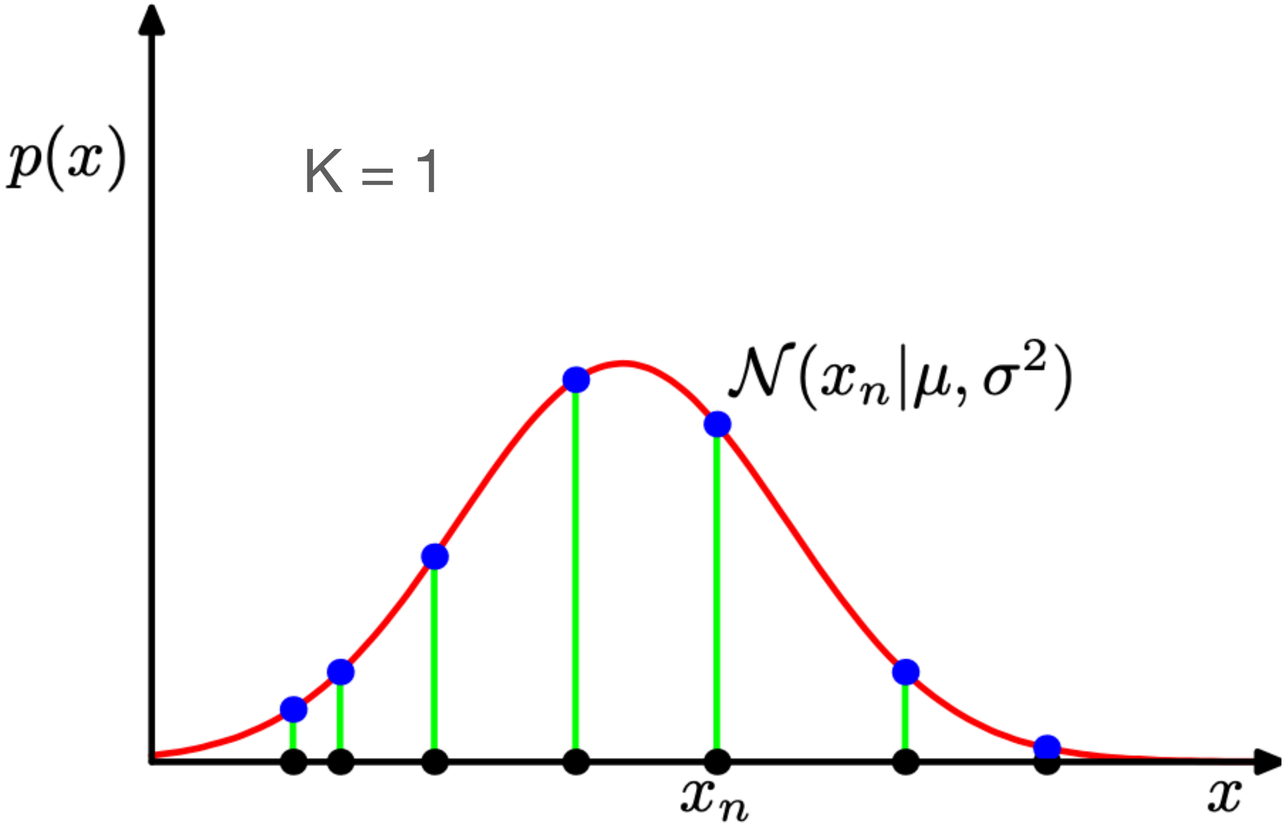
1. Derive covariance and mixture weight updates
2. Issues with maximum likelihood and workarounds
3. K-means as a special case
4. Theoretical foundation*: EM algorithm (1 is E step, 2 is M step)

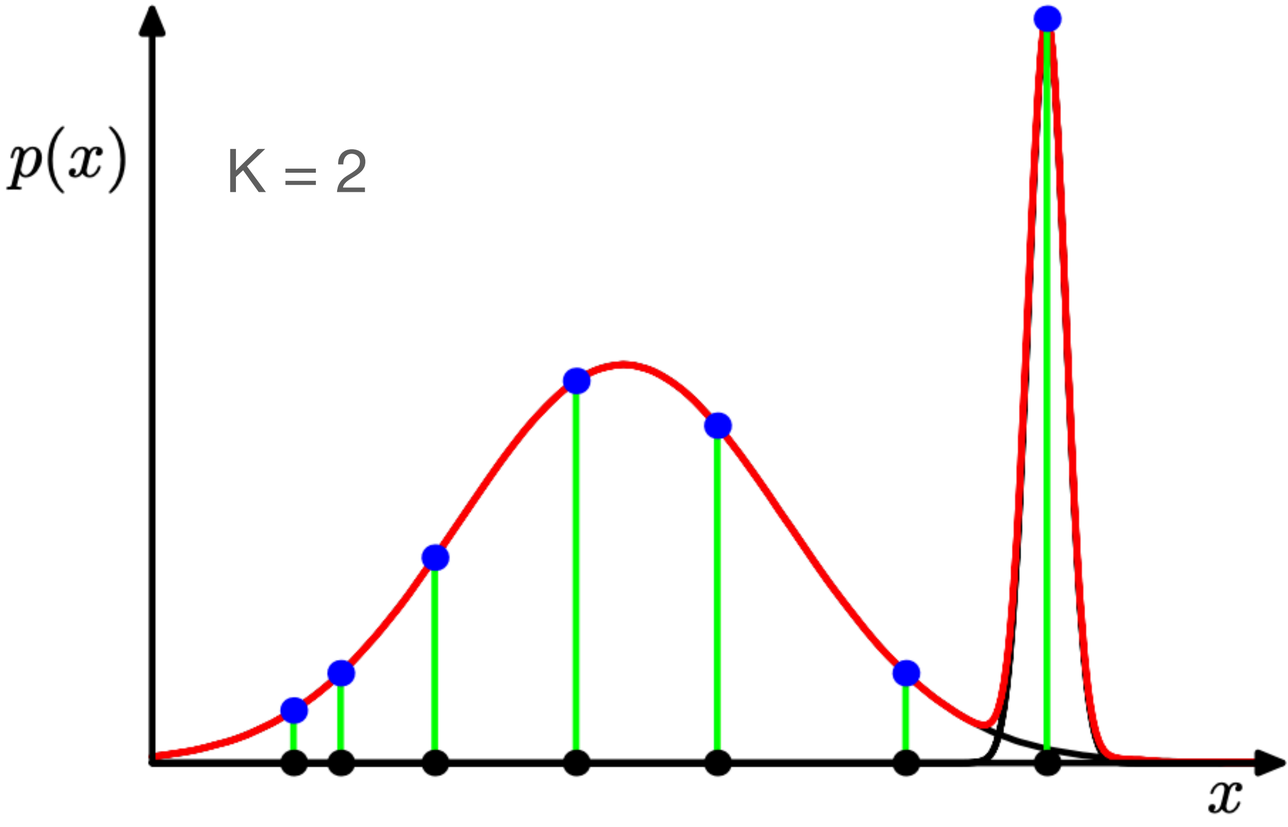
* not in assignment/exam

Maximum likelihood - overfitting

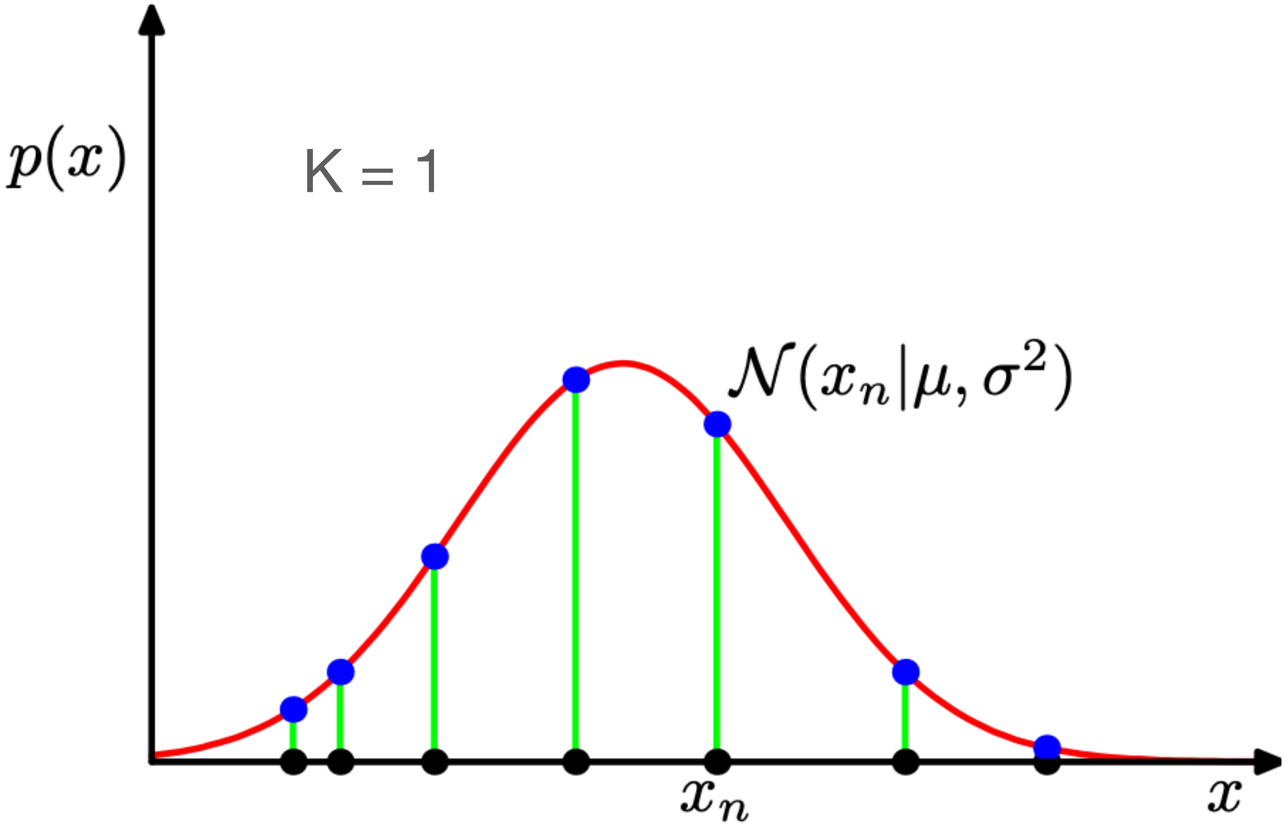


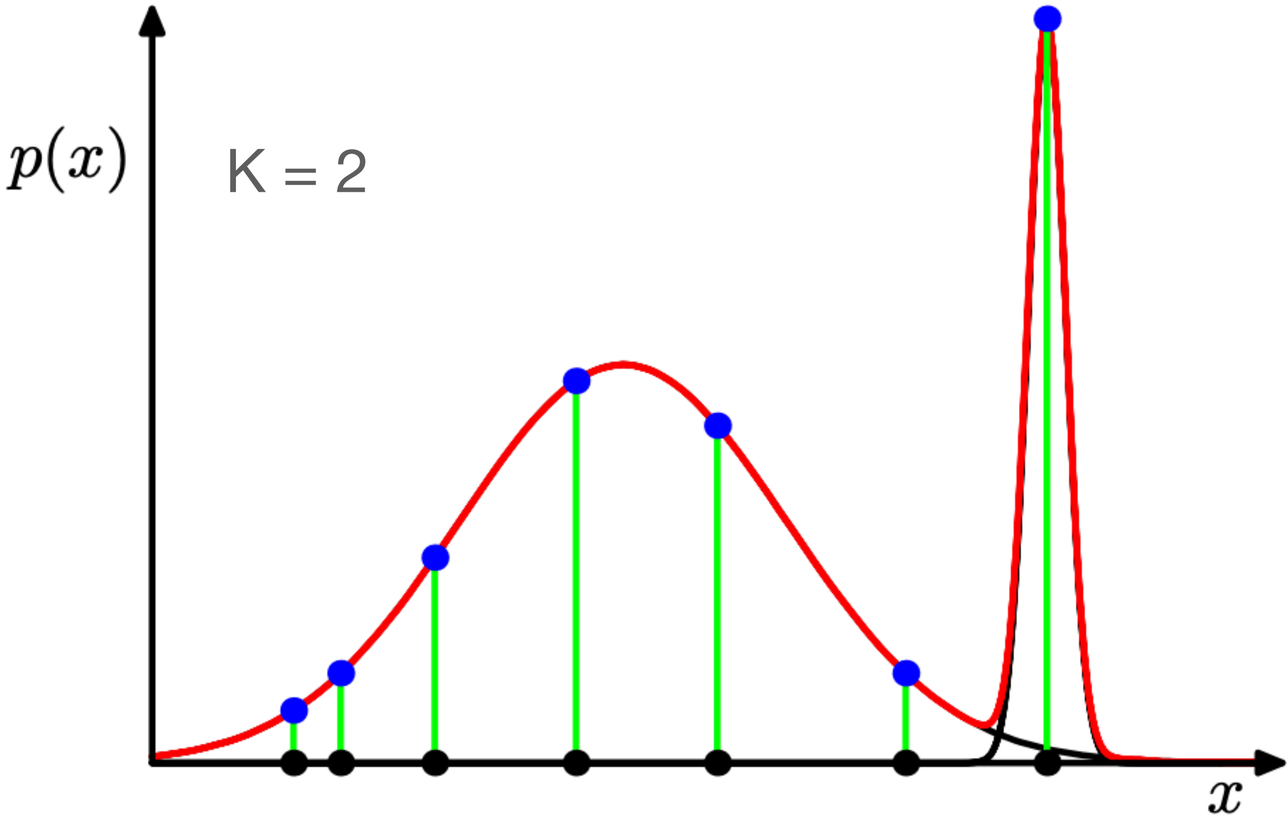
Maximum likelihood - overfitting





Maximum likelihood - overfitting

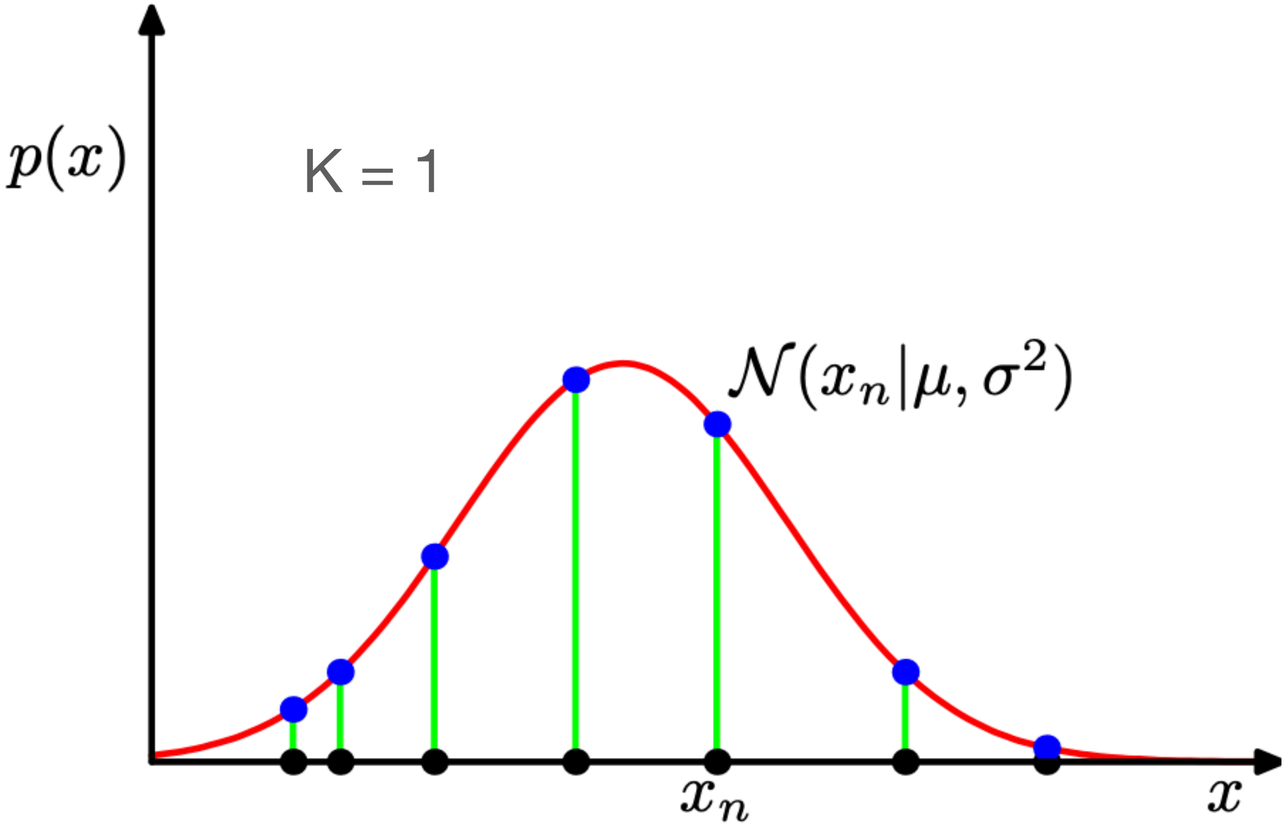


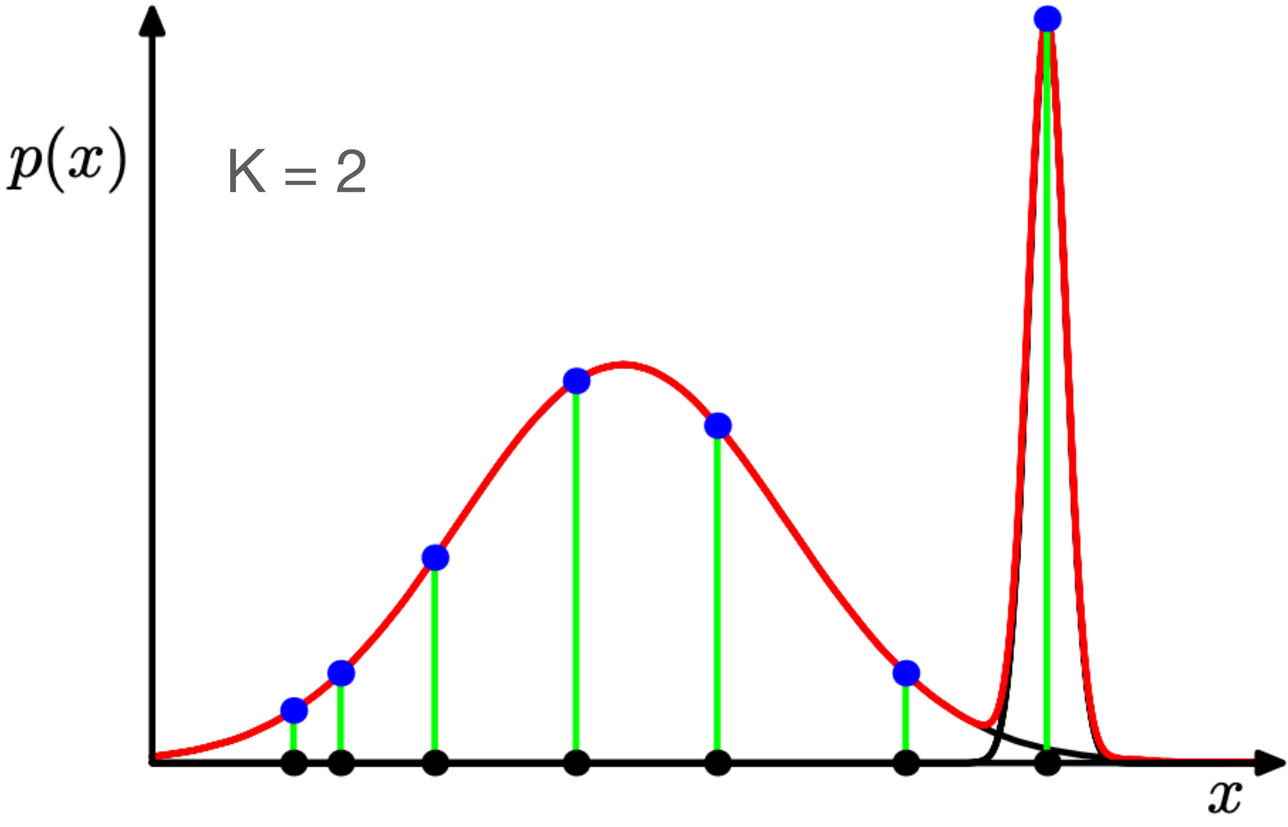


$$p_2(x_7 \,|\, \mu_2, \sigma_2^2) = \mathcal{N}(x_7; x_7, \sigma_2^2) = \frac{1}{\sqrt{2\pi}} \frac{1}{\sigma_2}$$

One component collapses to a data point!

Maximum likelihood - overfitting



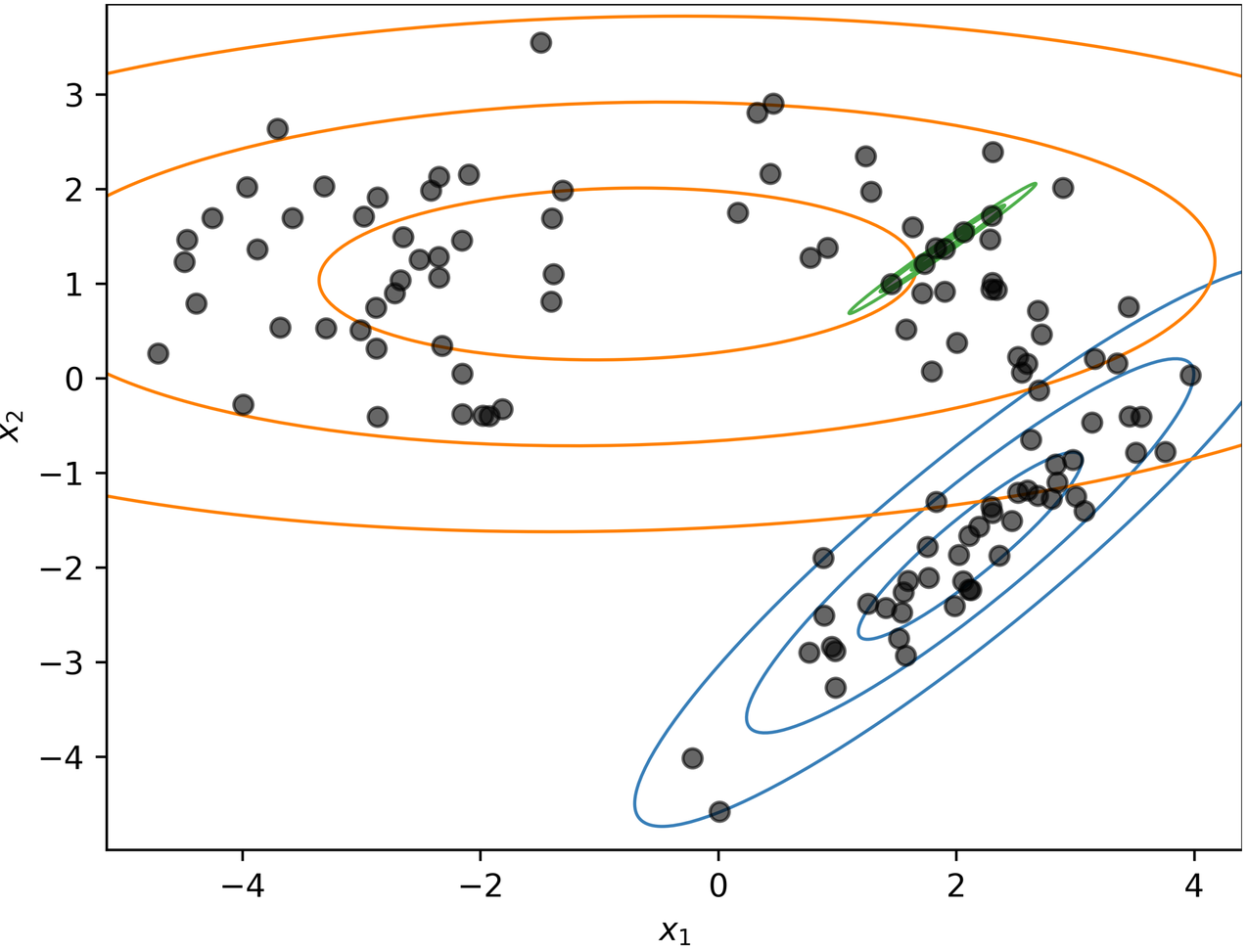


Hot-fix: reset the mean to a randomly chosen value, and the covariance to some large value and hope we don't have to reset again ¯_(ツ)_/¯

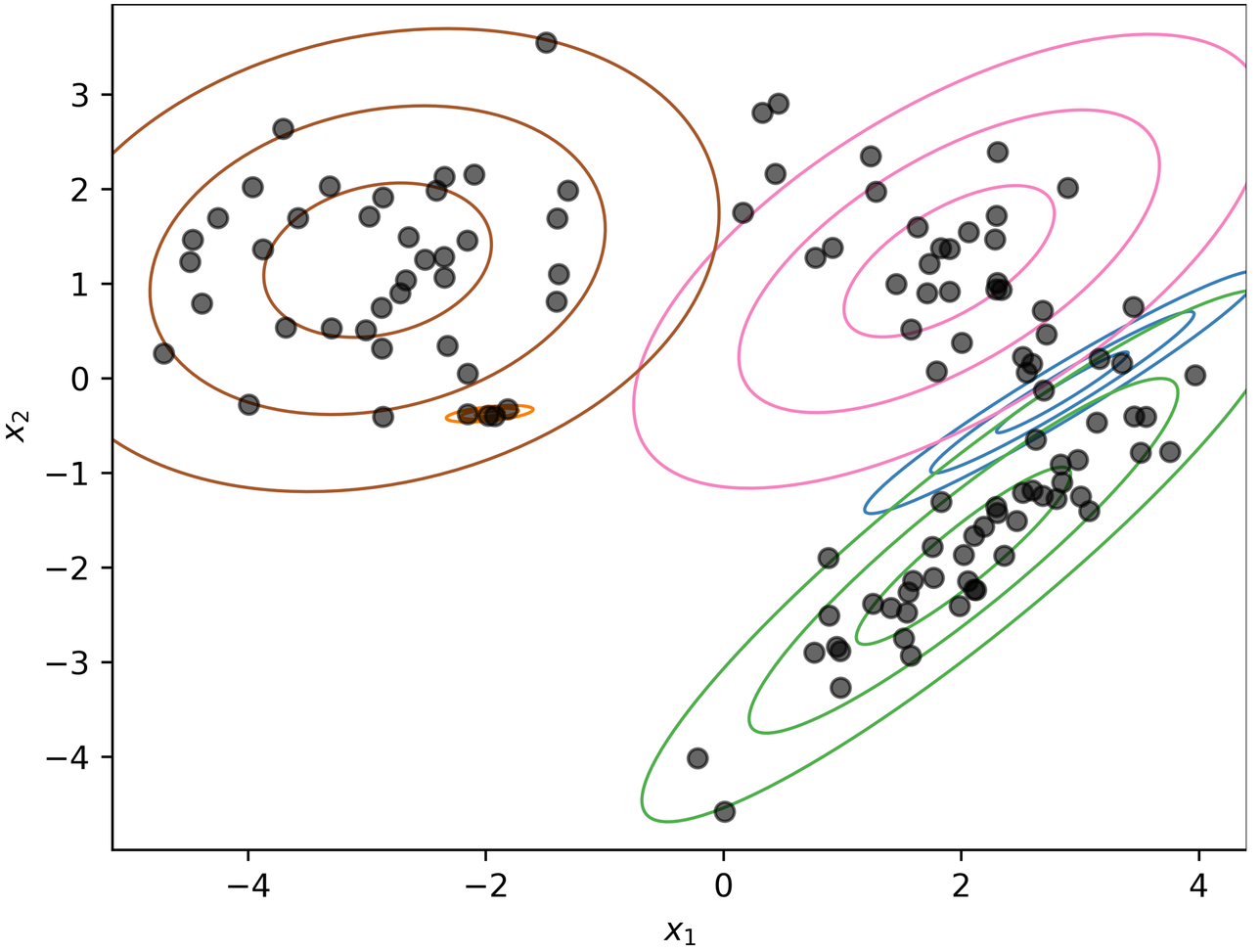
$$p_2(x_7 \,|\, \mu_2, \sigma_2^2) = \mathcal{N}(x_7; x_7, \sigma_2^2) = \frac{1}{\sqrt{2\pi}} \frac{1}{\sigma_2}$$

One component collapses to a data point!

Local minima

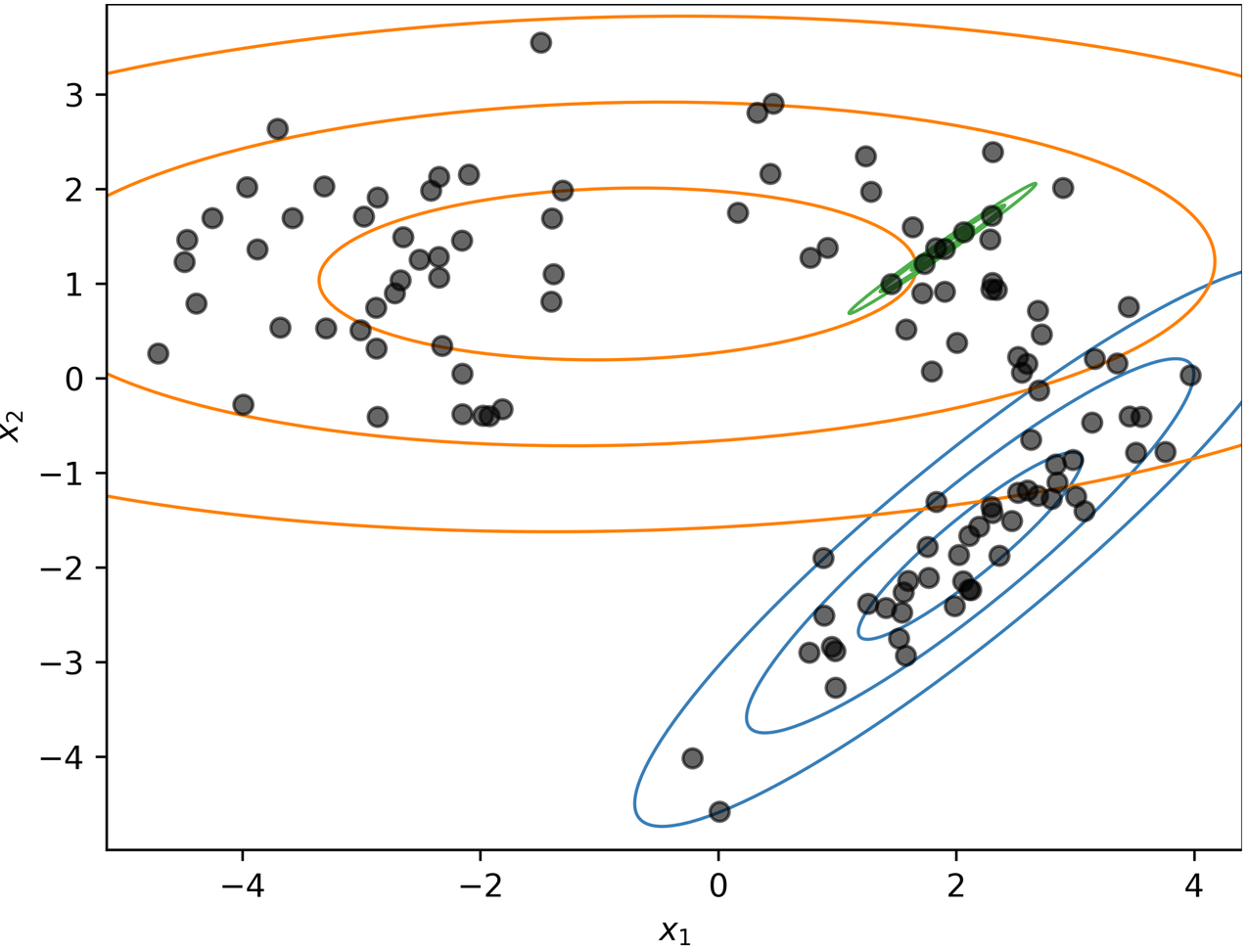


K = 3



K = 5

Local minima



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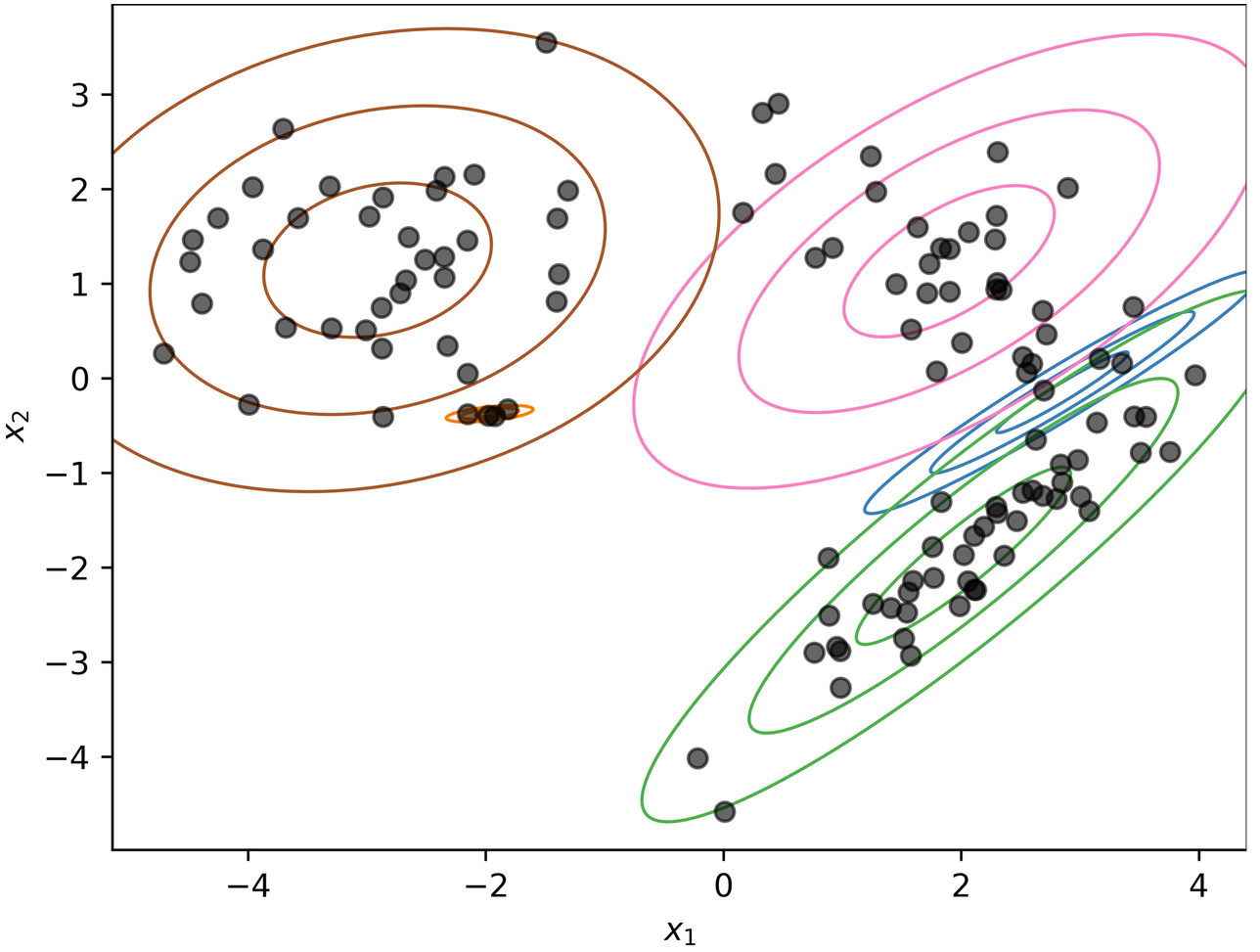

K = 5

Practical initialisation: k-means, mean/cov = sample mean/cov, mixture weights = proportions

Overview

Last lecture:

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Initialise $\{\pi_k, \mu_k, \Sigma_k\}_{k=1}^K$

Repeat until convergence:

1. **Evaluate responsibilities** r_{nk} for every data point x_n using current parameters:

$$r_{nk} = \frac{\pi_k \mathcal{N}(x_n; \mu_k, \Sigma_k)}{\sum_{j=1}^K \pi_j \mathcal{N}(x_n; \mu_j, \Sigma_j)}$$

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Relation to k-means

$$r_{nk} = \frac{\pi_k \mathcal{N}(x_n; \mu_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(x_n; \mu_j, \Sigma_j)}$$

Assume $\Sigma_1 = \Sigma_2 = \ldots = \Sigma_K = \epsilon \mathrm{I}$

Numerical example: $x_n = 5$, K = 3

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Numerical example: $x_n = 5$, K = 3

μ_k	π_k	$\pi_k \mathcal{N}(x_n; \mu_k, \Sigma_k)$	r_{nk}
8	0.3	0.02	0.27
-2	0.4	0.00016	0.01
4	0.3	0.0528	0.72

Soft assignment

$\epsilon = 4$

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4	0.3	0.0528	0.72

Soft assignment

$\epsilon = 4$

μ_k	π_k	$\pi_k \mathcal{N}(x_n; \mu_k, \Sigma_k)$	r_{nk}
8	0.3	0.44×10^{-195}	0
-2	0.4	1.5×10^{-1064}	0
4	0.3	0.23×10^{-22}	1

Hard assignment

$\epsilon = 0.01$

Overview

Last lecture:

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Initialise $\{\pi_k, \mu_k, \Sigma_k\}_{k=1}^K$

Repeat until convergence:

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* not in assignment/exam

GMMs - iterative procedure = *EM* algorithm

Initialise $\{\pi_k, \mu_k, \Sigma_k\}_{k=1}^K$

Repeat until convergence:

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$$r_{nk} = \frac{\pi_k \mathcal{N}(x_n; \mu_k, \Sigma_k)}{\sum_{j=1}^K \pi_j \mathcal{N}(x_n; \mu_j, \Sigma_j)}$$

E step

2. **Re-estimate parameters** $\{\pi_k, \mu_k, \Sigma_k\}_{k=1}^K$ using the current responsibilities r_{nk}:

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$$\pi_k = \frac{N_k}{N}$$

M step

Expectation maximisation (EM) algorithm*

Log-likelihood: $L(\theta) = \log p(X \mid \theta) = \sum_{n=1}^{N} \log p(x_n \mid \theta) = \sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k \mathcal{N}(x_n; \mu_k, \Sigma_k)$

Goal: maximum likelihood, $\operatorname{argmax}_\theta \; p(X \mid \theta)$, which is equivalent to $\operatorname{argmax}_\theta \; \log p(X \mid \theta)$

Assume: **latent/unknown/hidden variables** $\{z_n\}_{n=1}^{N}$ representing *component assignment*

$$L(\theta) = \log p(X \mid \theta) = \log \int p(X, z \mid \theta) \, \mathrm{d}z = \log \int q(z) \frac{p(X, z \mid \theta)}{q(z)} \, \mathrm{d}z \geq \int q(z) \log \frac{p(X, z \mid \theta)}{q(z)} \, \mathrm{d}z := \mathscr{F}(q(z), \theta)$$

An arbitrary $q(z)$ — Jensen's inequality — Lower bound on $L(\theta)$

Instead of maximising $L(\theta)$ directly, we will maximise the lower bound $\mathscr{F}(q(z), \theta)$, alternating between $q(z)$ and θ while keeping the other fixed.

EM for GMMs

1. **Evaluate responsibilities** r_{nk} for every data point x_n using current parameters:

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E step

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M step

EM for GMMs

Maximising lower bound wrt $q(z)$
whilst keeping θ fixed

$$q(z)^{(t+1)} \leftarrow \text{argmax}_{q(z)}\, \mathcal{F}(q(z), \theta^{(t)}) = p(z \mid X, \theta^{(t)})$$

fill in values for the hidden variables according to their posterior probabilities

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E step

Maximising lower bound wrt θ whilst keeping $q(z)$ fixed

$$\theta^{(t+1)} \leftarrow \text{argmax}_{\theta}\, \mathcal{F}(q(z)^{t+1}, \theta)$$

learn model as if hidden variables were not hidden

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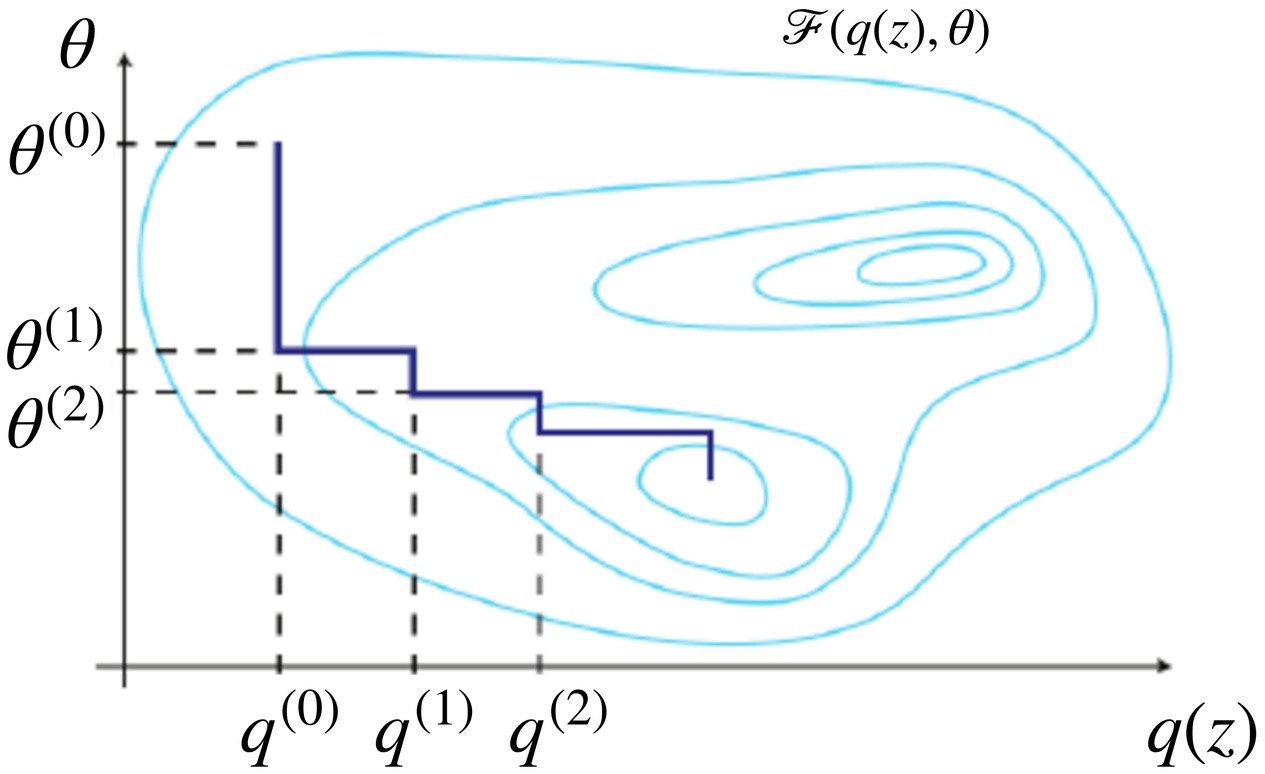
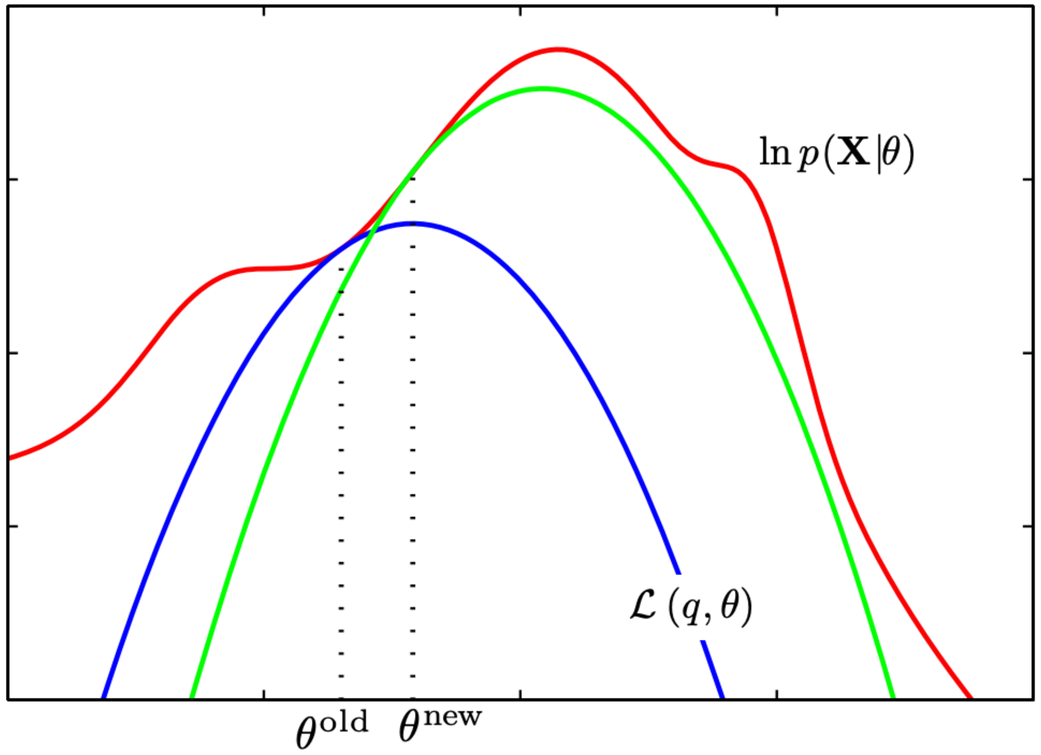
M step

EM algorithm - visualisation





EM algorithm - more visualisation

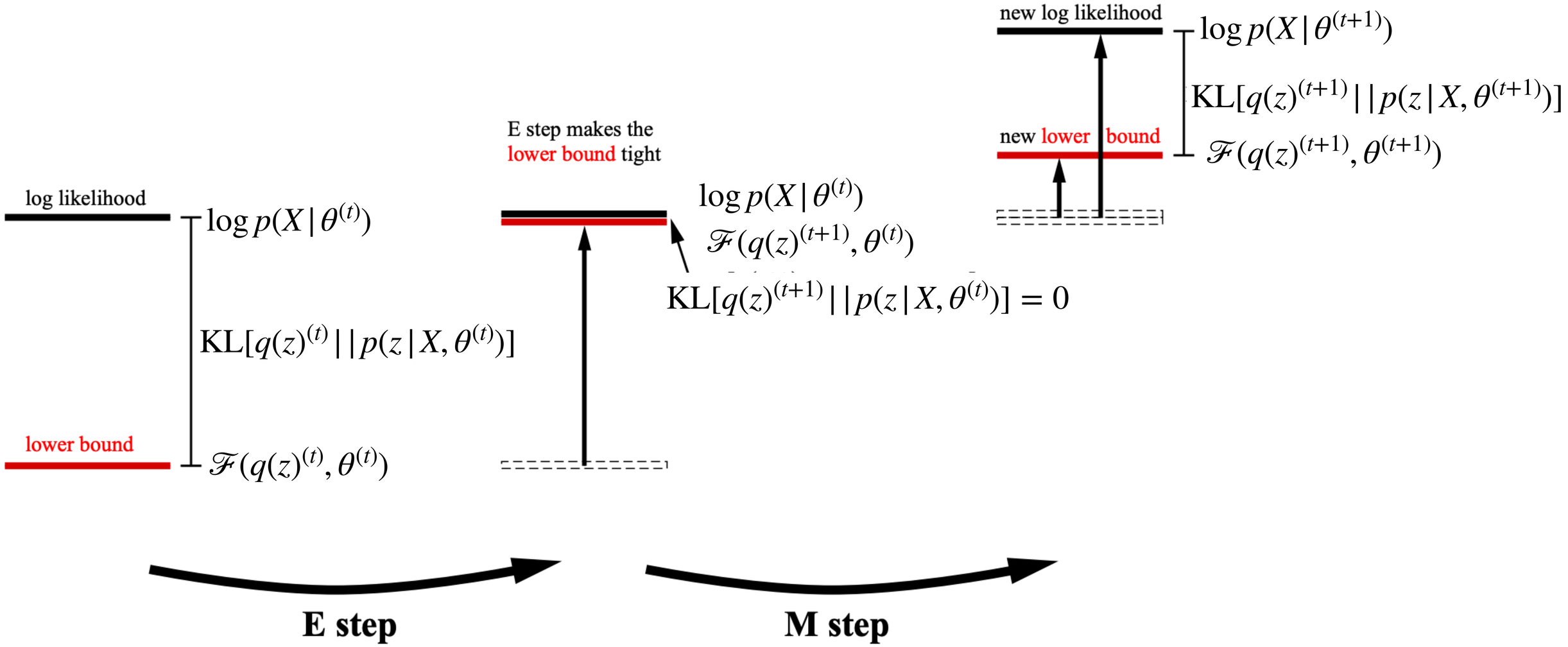


Figure credit: Beal (2003), Variational Algorithms for Approximate Bayesian Inference

Gaussian mixture models: check your understanding

Model: $$p_\theta(x) = \sum_{k=1}^{K} \pi_k \mathcal{N}(x; \mu_k, \Sigma_k) \qquad 0 \leq \pi_k \leq 1, \sum_{k=1}^{K} \pi_k = 1$$

where we defined $\theta = \{\pi_k, \mu_k, \Sigma_k \text{ for } k = 1,2,\ldots,K\}$ as the parameters of the GMM.

- If K takes a greater value, the likelihood becomes greater after convergence.
- Assume we have N data points. The maximum likelihood will be achieved if we set $K = N$.
- In GMM, the EM algorithm gives us *global* minimum, because we can update π_k, μ_k, and Σ_k through closed-form solutions.
- GMM has a higher computational complexity than k-means.

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where we defined $\theta = \{\pi_k, \mu_k, \Sigma_k \text{ for } k = 1,2,\ldots,K\}$ as the parameters of the GMM.

- If K takes a greater value, the likelihood becomes greater after convergence. Yes
- Assume we have N data points. The maximum likelihood will be achieved if we set $K = N$.
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- GMM has a higher computational complexity than k-means.

Gaussian mixture models: check your understanding

Model: $$p_\theta(x) = \sum_{k=1}^{K} \pi_k \mathcal{N}(x; \mu_k, \Sigma_k) \qquad 0 \leq \pi_k \leq 1, \sum_{k=1}^{K} \pi_k = 1$$

where we defined $\theta = \{\pi_k, \mu_k, \Sigma_k \text{ for } k = 1,2,\ldots,K\}$ as the parameters of the GMM.

- If K takes a greater value, the likelihood becomes greater after convergence. Yes
- Assume we have N data points. The maximum likelihood will be achieved if we set $K = N$. Yes
- In GMM, the EM algorithm gives us *global* minimum, because we can update π_k, μ_k, and Σ_k through closed-form solutions.
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Overview

Last lecture:

1. **Model**: Gaussian mixture models
2. **Learning**: parameter learning using *maximum likelihood*
3. **Iterative** procedure, derive mean update

Initialise $\{\pi_k, \mu_k, \Sigma_k\}_{k=1}^K$

Repeat until convergence:

1. **Evaluate responsibilities** r_{nk} for every data point x_n using current parameters:

$$r_{nk} = \frac{\pi_k \mathcal{N}(x_n; \mu_k, \Sigma_k)}{\sum_{j=1}^K \pi_j \mathcal{N}(x_n; \mu_j, \Sigma_j)}$$

2. **Re-estimate parameters** $\{\pi_k, \mu_k, \Sigma_k\}_{k=1}^K$ using the current responsibilities r_{nk}:

$$\mu_k = \frac{1}{N_k} \sum_{n=1}^N r_{nk} x_n, \quad N_k = \sum_{n=1}^N r_{nk}$$

$$\Sigma_k = \frac{1}{N_k} \sum_{n=1}^N r_{nk} (x_n - \mu_k)(x_n - \mu_k)^\intercal$$

$$\pi_k = \frac{N_k}{N}$$

This lecture:

1. Derive covariance and mixture weight updates
2. Issues with maximum likelihood and workarounds
3. K-means as a special case
4. Theoretical foundation*: EM algorithm (1 is E step, 2 is M step)

* not in assignment/exam