Lecture 2: Frequency Vs. Bayes

Reading: Sections 2.4, 8.3

GU4241/GR5241 Statistical Machine Learning

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Parametric Models

Models

A **model** $\mathcal{P}$ is a set of probability distributions. We index each distribution by a parameter value $\theta \in \mathcal{T}$; we can then write the model as

$$\mathcal{P} = \{P_\theta | \theta \in \mathcal{T}\} .$$

The set $\mathcal{T}$ is called the **parameter space** of the model.

Parametric model

The model is called **parametric** if the number of parameters (i.e. the dimension of the vector θ) is (1) finite and (2) independent of the number of data points. Intuitively, the complexity of a parametric model does not increase with sample size.

Density representation

For parametric models, we can assume that $\mathcal{T} \subset \mathbb{R}^d$ for some fixed dimension d. We usually represent each P_θ be a density function $p(x|\theta)$.

Maximum Likelihood Estimation

Setting

- Given: Data $x_1, \ldots, x_n$, parametric model $\mathcal{P} = \{p(x|\theta) \,|\, \theta \in \mathcal{T}\}$.
- Objective: Find the distribution in $\mathcal{P}$ which best explains the data. That means we have to choose a "best" parameter value $\hat{\theta}$.

Maximum Likelihood approach

Maximum Likelihood assumes that the data is best explained by the distribution in $\mathcal{P}$ under which it has the highest probability (or highest density value).

Hence, the **maximum likelihood estimator** is defined as

$$\hat{\theta}_{ML} := \arg\max_{\theta \in \mathcal{T}} p(x_1, \ldots, x_n|\theta)$$

the parameter which maximizes the joint density of the data.

Analytic Maximum Likelihood

The i.i.d. assumption

The standard assumption of ML methods is that the data is **independent and identically distributed (i.i.d.)**, that is, generated by independently sampling repeatedly from the same distrubtion P.

If the density of P is $p(x|\theta)$, that means the joint density decomposes as

$$p(x_1, \ldots, x_n) = \prod_{i=1}^{n} p(x_i|\theta)$$

Maximum Likelihood equation

The analytic criterion for a maximum likelihood estimator (under the i.i.d. assumption) is:

$$\nabla_\theta \Big(\prod_{i=1}^{n} p(x_i|\theta) \Big) = 0$$

We use the "logarithm trick" to avoid a huge product rule computation.

Logarithm Trick

Recall: Logarithms turn products into sums

$$\log\Big(\prod_i f_i\Big) = \sum_i \log(f_i)$$

Logarithms and maxima

The logarithm is monotonically increasing on $\mathbb{R}_+$.

Consequence: Application of $\log$ does not change the *location* of a maximum or minimum:

$$\max_y \log(g(y)) \neq \max_y g(y) \qquad \text{The } \textit{value} \text{ changes.}$$

$$\arg\max_y \log(g(y)) = \arg\max_y g(y) \qquad \text{The } \textit{location} \text{ does not change.}$$

Analytic MLE

Likelihood and logarithm trick

$$\begin{aligned}\hat{\theta}_{ML} &= \arg\max_{\theta} \prod_{i=1}^{n} p(x_i|\theta) &&= \arg\max_{\theta} \log\Big(\prod_{i=1}^{n} p(x_i|\theta)\Big) \\ &&&= \arg\max_{\theta} \sum_{i=1}^{n} \log p(x_i|\theta)\end{aligned}$$

Analytic maximality criterion

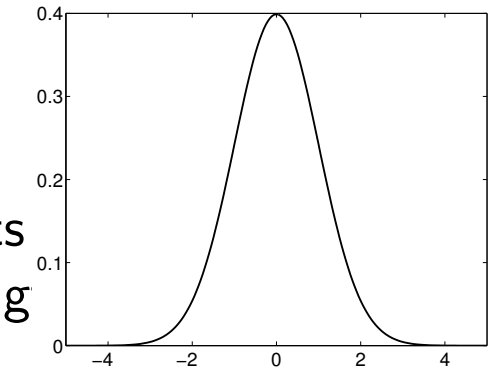
$$0 = \sum_{i=1}^{n} \nabla_\theta \log p(x_i|\theta) = \sum_{i=1}^{n} \frac{\nabla_\theta p(x_i|\theta)}{p(x_i|\theta)}$$

Whether or not we can solve this analytically depends on the choice of the model!

Example: Gaussian Mean MLE

Gaussian density in one dimension

$$g(x;\mu,\sigma) := \frac{1}{\sqrt{2\pi}\sigma}\exp\Big(-\frac{(x-\mu)^2}{2\sigma^2}\Big)$$

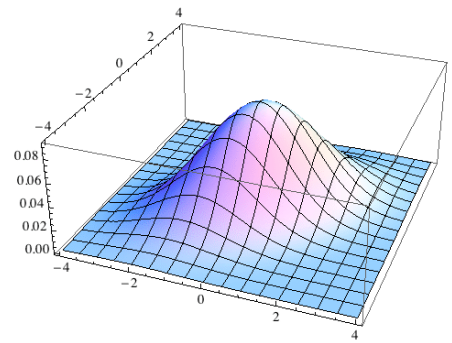


- The quotient $\frac{x-\mu}{\sigma}$ measures deviation of x from its expected value in units of σ (i.e. σ defines the leng scale)

Gaussian density in d dimensions

The quadratric function

$$-\frac{(x-\mu)^2}{2\sigma^2} \quad = \quad -\frac{1}{2}(x-\mu)(\sigma^2)^{-1}(x-\mu)$$



is replaced by a quadratic form:

$$g(\mathbf{x};\boldsymbol{\mu},\Sigma) := \frac{1}{\sqrt{(2\pi)^d\det(\Sigma)}}\exp\Big(-\frac{1}{2}\left\langle(\mathbf{x}-\boldsymbol{\mu}),\Sigma^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\rangle\Big)$$

Example: Gaussian Mean MLE

Model: Multivariate Gaussians

The model $\mathcal{P}$ is the set of all Gaussian densities on $\mathbb{R}^d$ with *fixed* covariance matrix Σ,

$$\mathcal{P} = \{g(\,.\,|\mu, \Sigma) \,|\, \mu \in \mathbb{R}^d\}\,,$$

where g is the Gaussian density function. The parameter space is $\mathcal{T} = \mathbb{R}^d$.

MLE equation

We have to solve the maximum equation

$$\sum_{i=1}^{n} \nabla_\mu \log g(x_i|\mu, \Sigma) = 0$$

for μ.

Example: Gaussian Mean MLE

$$
\begin{aligned}
0 &= \sum_{i=1}^{n} \nabla_\mu \log \frac{1}{\sqrt{(2\pi)^d |\Sigma|}} \exp\Big(-\frac{1}{2}\left\langle (x_i-\mu), \Sigma^{-1}(x_i-\mu)\right\rangle\Big) \\
&= \sum_{i=1}^{n} \nabla_\mu \Big(\log\Big(\frac{1}{\sqrt{(2\pi)^d |\Sigma|}}\Big) + \log\Big(\exp\Big(-\frac{1}{2}\left\langle (x_i-\mu), \Sigma^{-1}(x_i-\mu)\right\rangle\Big)\Big) \\
&= \sum_{i=1}^{n} \nabla_\mu \Big(-\frac{1}{2}\left\langle (x_i-\mu), \Sigma^{-1}(x_i-\mu)\right\rangle\Big) = -\sum_{i=1}^{n} \Sigma^{-1}(x_i-\mu)
\end{aligned}
$$

Multiplication by $(-\Sigma)$ gives

$$
0 = \sum_{i=1}^{n} (x_i - \mu) \qquad \Rightarrow \qquad \mu = \frac{1}{n}\sum_{i=1}^{n} x_i
$$

Conclusion

The maximum likelihood estimator of the Gaussian expectation parameter for fixed covariance is

$$
\hat{\mu}_{\mathsf{ML}} := \frac{1}{n}\sum_{i=1}^{n} x_i
$$

Example: Gaussian with Unknown Covariance

Model: Multivariate Gaussians

The model $\mathcal{P}$ is now

$$\mathcal{P} = \{g(\,.\,|\mu, \Sigma) \,|\, \mu \in \mathbb{R}^d, \Sigma \in \Delta_d\}\ ,$$

where Δ_d is the set of positive definite $d \times d$-matrices. The parameter space is $\mathcal{T} = \mathbb{R}^d \times \Delta_d$.

ML approach

Since we have just seen that the ML estimator of μ does not depend on Σ, we can compute $\hat{\mu}_{\mathsf{ML}}$ first. We then estimate Σ using the criterion

$$\sum_{i=1}^{n} \nabla_\Sigma \log g(x_i|\hat{\mu}_{\mathsf{ML}}, \Sigma) = 0$$

Solution

The ML estimator of Σ is

$$\hat{\Sigma}_{\mathsf{ML}} := \frac{1}{n}\sum_{i=1}^{n}(x_i - \hat{\mu}_{\mathsf{ML}})(x_i - \hat{\mu}_{\mathsf{ML}})^t\ .$$

Bayesian models

The defining assumption of **Bayesian statistics** is that the distribution P_θ which models the data is a random quantity and itself has a distribution Q. The generative model for data $X_1, X_2, \ldots$ is

$$\begin{aligned} P_\theta &\sim Q \\ X_1, X_2, \ldots &\overset{i.i.d.}{\sim} P_\theta \end{aligned}$$

The rational behind the approach is:

- In any statistical approach (Bayesian or frequentist), the distribution P_θ is unknown.
- Bayesian statistics argues that any form of uncertainty should be expressed by probability distributions.
- We can think of the randomness in Q as a model of the statistician's lack of knowledge regarding P_θ.

Prior and posterior

The distribution Q of P_θ is called the **a priori distribution** (or the **prior** for short). We use q to denote its density if it exists.

Our objective is to determine the conditional probability of P given observed data

$$\Pr(\theta|x_1, \ldots, x_n).$$

The distribution is called the **a posteriori distribution** or **posterior**.

Bayes' Theorem

Given data $X_1, \ldots, X_n$, we can compute the posterior by

$$\Pr(\theta|x_1, \ldots, x_n) = \frac{(\prod_{i=1}^n p(x_i|\theta))q(\theta)}{p(x_1, \ldots, x_n)} = \frac{(\prod_{i=1}^n p(x_i|\theta))q(\theta)}{\int (\prod_{i=1}^n p(x_i|\theta))\, q(\theta)}.$$

The individual terms have names:

$$\text{posterior} = \frac{\text{likelihood} \times \text{prior}}{\text{evidence}}$$

Example: unknown Gaussian mean

Model

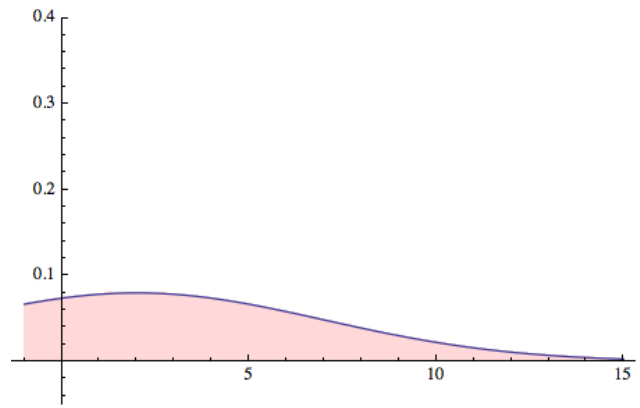
We assume that the data is generated from a Gaussian with fixed variance σ^2. The mean μ is unknown. The model likelihood is $p(x|\mu, \sigma) = g(x|\mu, \sigma)$ (where g is the Gaussian density on the line).

Bayesian model

We choose a Gaussian prior on μ,

$$q(\mu) := g(\mu|\mu_0, \sigma_0) \ .$$

In the figure, $\mu_0 = 2$ and $\sigma_0 = 5$. Hence, we assume that $\mu_0 = 2$ is the most probable value of μ, and that $\mu \in [-3, 7]$ with a probability ~ 0.68.



Example: unknown Gaussian mean

Application of Bayes' formula to the Gaussian-Gaussian model shows the posterior distribution is

$$\Pr(\mu|x_{1:n}) = g(\mu|\mu_n, \sigma_n),$$

where $\mu_n := \frac{\sigma^2\mu_0 + \sigma_0^2 \sum_{i=1}^n x_i}{\sigma^2 + n\sigma_0^2}$ and $\sigma_n^2 := \frac{\sigma^2\sigma_0^2}{\sigma^2 + n\sigma_0^2}$.

Example: unknown Gaussian mean

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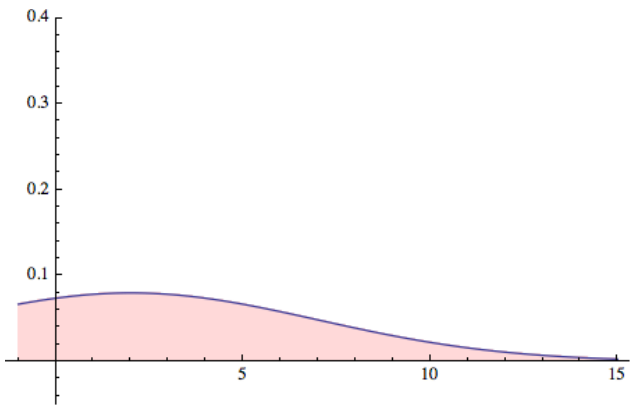
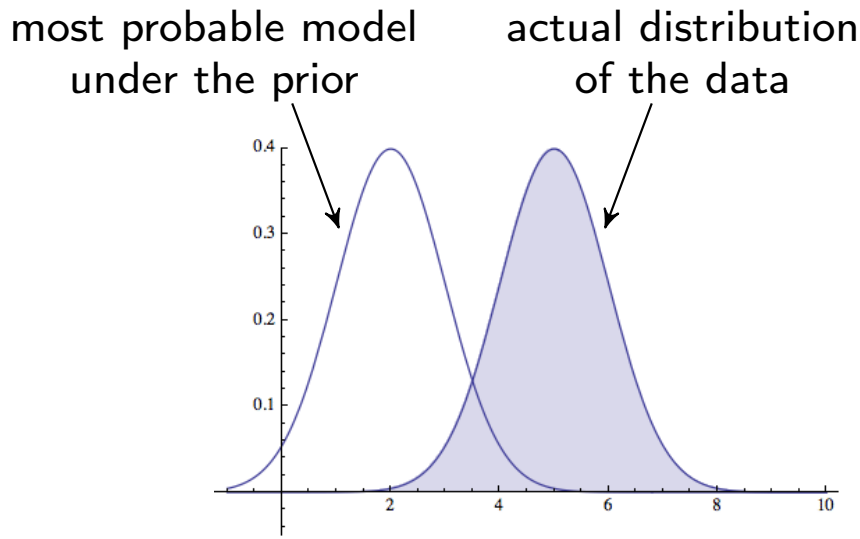


Prior



Sampling distribution

Example: unknown Gaussian mean

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$$\Pr(\mu|x_{1:n}) = g(\mu|\mu_n, \sigma_n),$$

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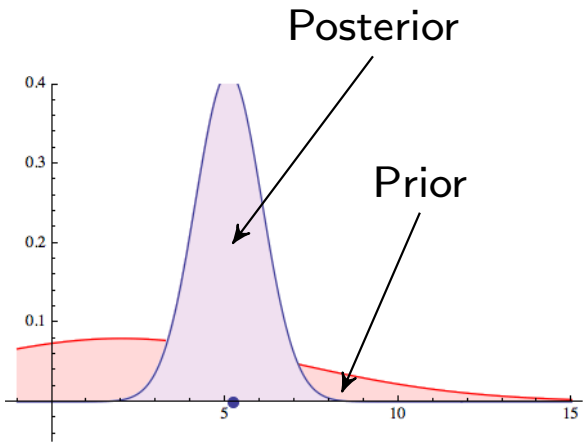
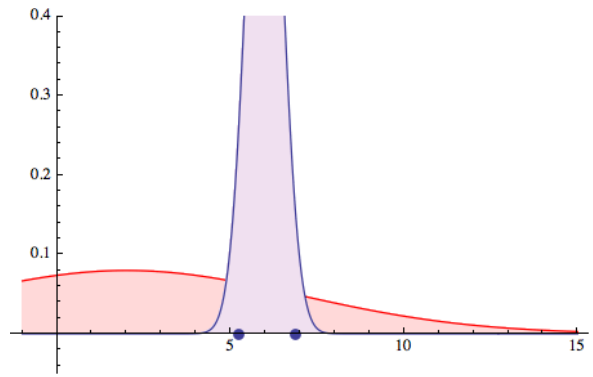
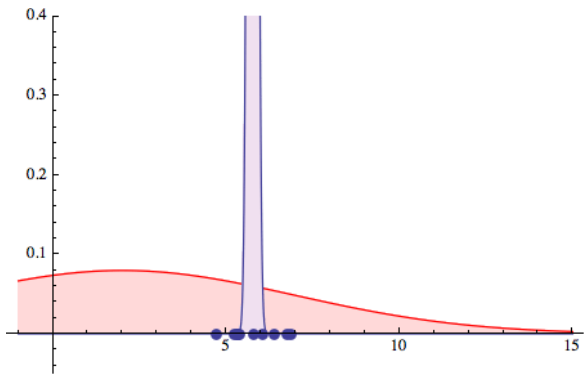


$n = 1$



$n = 2$



$n = 10$

MAP estimation

Suppse $\Pi(\theta|x_{1:n})$ is the posterior of a Bayesian model. The estimator

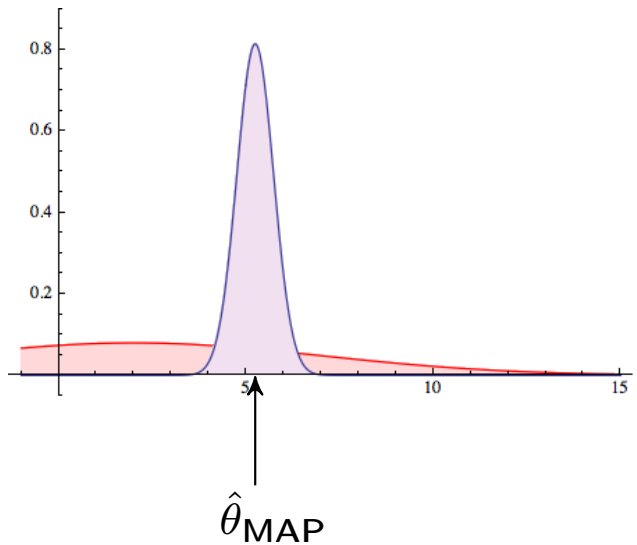
$$\hat{\theta}_{\mathsf{MAP}} = \arg\max_{\theta} \Pi(\theta|x_{1:n})$$

is called the **maximum a posteriori** (or **MAP**) estimator for θ.

Point estimates

The goal of Bayesian inference is to compute the posterior distribution. Contrast this to classical statistics (e.g. maximum likelihood), where we typically estimate a single value for θ (a so-called **point estimate**).

MAP estimation combines aspects of Bayesian methodology (use of a prior) with aspects of classical methodology (since $\hat{\theta}_{\mathsf{MAP}}$ is a point estimate).



MAP and regularization

Logarithmic view

Since the logarithm leaves the maximum invariant,

$$\hat{\theta}_{\mathsf{MAP}} = \arg\max_{\theta} \Pi(\theta|x_{1:n}) = \arg\max_{\theta} \log \Pi(\theta|x_{1:n})$$

Substituting in the Bayes equation gives

$$\log \Pi(\theta|x_{1:n}) = \sum_{i=1}^{n} \log p(x_i|\theta) + \log q(\theta) - \log p(x_1, \ldots, x_n) \ .$$

MAP as regularized ML

Since log-evidence does not depend on θ,

$$\hat{\theta}_{\mathsf{MAP}} = \arg\max_{\theta} \Big\{ \sum_{i=1}^{n} \log p(x_i|\theta) + \log q(\theta) \Big\}$$

Thus, the MAP estimate can be regarded as a regularized version of a maximum likelihood estimator. The regularization term $\log q(\theta)$ favors values where q (and hence $\log q$) is large.

Classification problems

In a classification setting, the output takes values in a discrete set.

For example, if we are predicting the brand of a car based on a number of variables, the function f takes values in the set
$\{$Ford, Toyota, Mercedes-Benz, $\dots\}$.

We will use slightly different notation:

$$P(X, Y) : \text{joint distribution of } (X, Y),$$
$$P(Y \mid X) : \text{conditional distribution of } X \text{ given } Y,$$
$$\hat{y}_i : \text{prediction for } x_i.$$

Loss function for classification

There are many ways to measure the error of a classification prediction. One of the most common is the 0-1 loss:

$$E(\mathbf{1}(y_0 \neq \hat{y}_0))$$

Like the MSE, this quantity can be estimated from training and test data by taking a sample average:

$$\frac{1}{n}\sum_{i=1}^{n}\mathbf{1}(y_i \neq \hat{y}_i)$$

Bayes classifier

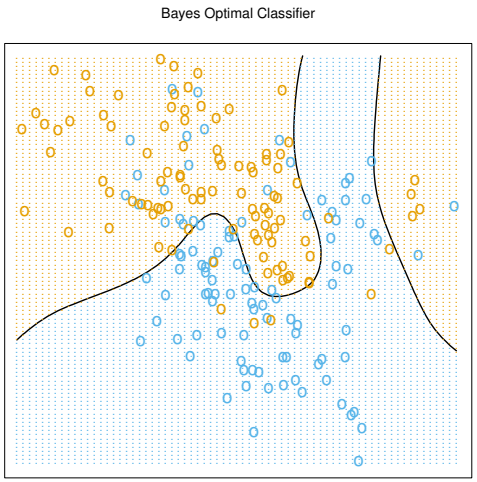


FIGURE 2.5. *The optimal Bayes decision boundary for the simulation example of Figures 2.1, 2.2 and 2.3. Since the generating density is known for each class, this boundary can be calculated exactly (Exercise 2.2).*

In practice, we never know the joint probability P. However, we can assume that it exists.

The Bayes classifier assigns:

$$\hat{y}_i = \text{argmax}_k \;\; P(Y = k \mid X = x_i)$$

It can be shown that this is the best classifier under the 0-1 loss.

Images of Linear Mappings (1)

Linear mapping

A matrix $\mathbf{X} \in \mathbb{R}^{n \times m}$ defines a linear mapping $f_{\mathbf{x}} : \mathbb{R}^m \to \mathbb{R}^n$.

Image

Recall: The **image** of a mapping f is the set of all possible function values, here

$$\text{image}(f_{\mathbf{x}}) := \{\mathbf{y} \in \mathbb{R}^n \mid \mathbf{Xz} = \mathbf{y} \text{ for some } \mathbf{z} \in \mathbb{R}^m\}$$

Image of a linear mapping

- The image of a linear mapping $\mathbb{R}^m \to \mathbb{R}^n$ is a linear subspace of $\mathbb{R}^n$.
- The columns of $\mathbf{X}$ form a basis of the image space:

$$\text{image}(\tilde{\mathbf{X}}) = \text{span}\{\mathbf{X}_1^{\text{col}}, \ldots, \mathbf{X}_m^{\text{col}}\}$$

- This is one of most useful things to remember about matrices, so, again:

The columns span the image.

Images of Linear Mappings (2)

Dimension of the image space

Clearly: The number of linearly independent column vectors. This number is called the **column rank** of $\mathbf{X}$.

Invertible mappings

Recall: A mapping f is invertible if it is one-to-one, i.e. for each function value $\tilde{\mathbf{y}}$ there is exactly one input value with $f(\mathbf{z}) = \tilde{\mathbf{y}}$.

Invertible matrices

The matrix $\tilde{\mathbf{X}}$ is called invertible if $f_{\mathbf{x}}$ is invertible.

- Only square matrices can be invertible.
- For a *linear* mapping: If $\tilde{\mathbf{X}}$ is a square matrix $f_{\mathbf{x}}$ is invertible iff the image has the same dimension as the input space.
- Even if $\tilde{\mathbf{X}} \in \mathbb{R}^{n \times m}$, the matrix $\tilde{\mathbf{X}}^t \tilde{\mathbf{X}}$ is in $\mathbb{R}^{m \times m}$ (a square matrix).
- So: $\tilde{\mathbf{X}}^t \tilde{\mathbf{X}}$ is invertible if $\tilde{\mathbf{X}}$ has full column rank.

Symmetric and Orthogonal Matrices

Recall: Transpose

The transpose A^T of a matrix $A \in \mathbb{R}^m$ is the matrix with entries

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

Orthogonal matrices

A matrix $O \in \mathbb{R}^{m \times m}$ is called **orthogonal**

$$O^{-1} = O^T$$

Orthogonal matrices describe two types of operations:

1. Rotations of the coordinate system.
2. Permutations of the coordinate axes.

Symmetric matrices

A matrix $A \in \mathbb{R}^{m \times m}$ is called **symmetric**

$$A = A^\mathsf{T}$$

Note: Symmetric and orthogonal matrices are very different objects. Only the identity is both.

Orthonormal Bases

Recall: ONB

A basis $\{v_1, \ldots, v_m\}$ of $\mathbb{R}^m$ is called an **orthonormal basis** if

$$\langle v_i, v_j \rangle = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

In other words, the v_i are pairwise orthogonal and each of length 1.

Orthogonal matrices

A matrix is orthogonal precisely if its rows form an ONB. Any two ONBs can be transformed into each other by an orthogonal matrix.

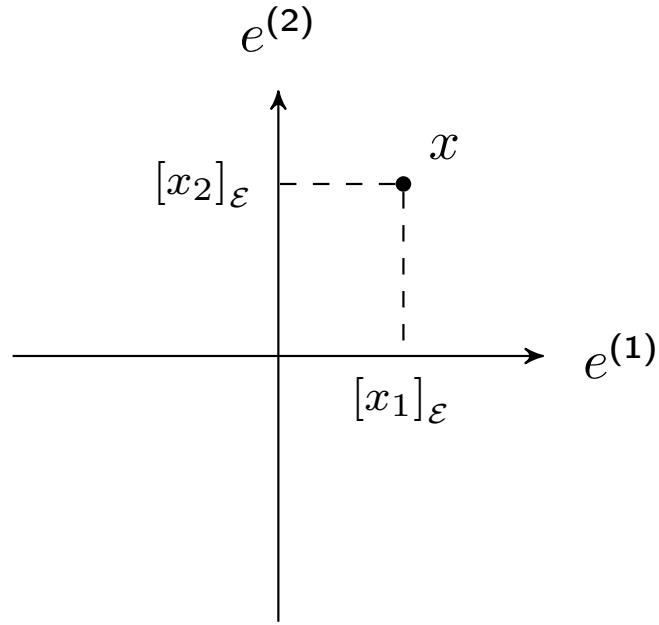
Basis representation

Representation of a vector

Suppose $\mathcal{E} = \{e_1, \ldots, e_d\}$ is a basis of a vector space. Then a vector x is represented as

$$x = \sum_{j=1}^{d} [x_j]_{\mathcal{E}} e^{(j)}$$

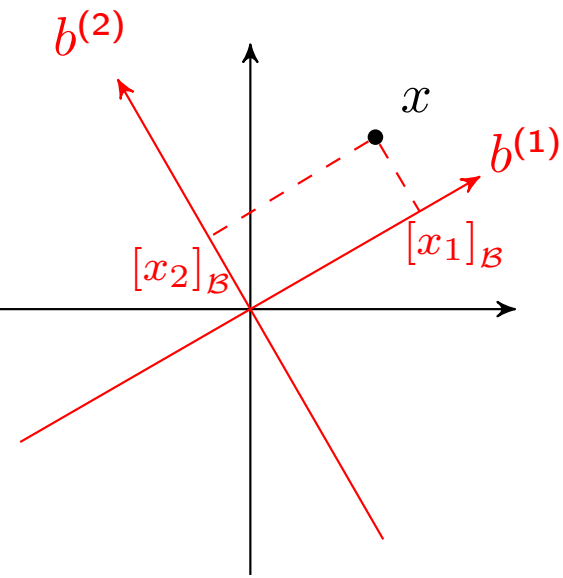
$[x_j]_{\mathcal{E}} \in \mathbb{R}$ are the coordinates of x w.r.t. $\mathcal{E}$.



Other bases

If $\mathcal{B} = \{b_1, \ldots, b_d\}$ is another basis, x can be represented alternatively as

$$x = \sum_{j=1}^{d} [x_j]_{\mathcal{B}} b^{(j)}$$



Changing bases

Change-of-basis matrix

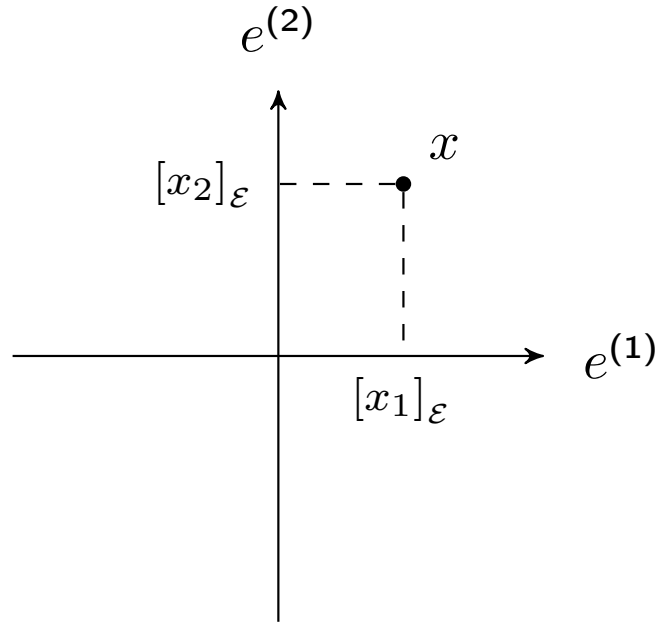
The matrix

$$M := \left([e^{(1)}]_{\mathcal{B}}, \ldots, [e^{(d)}]_{\mathcal{B}} \right)$$

transforms between the bases, i.e.

$$M[x]_{\mathcal{E}} = [x]_{\mathcal{B}} \ .$$

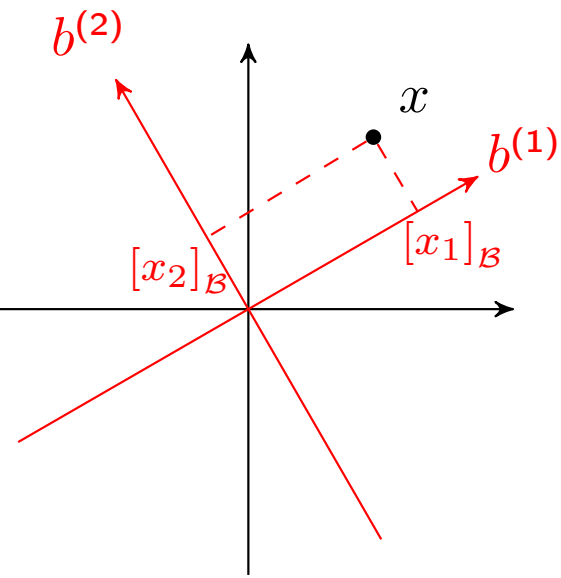
If both $\mathcal{E}$ and $\mathcal{B}$ are ONBs, M is orthogonal.



Representation of matrices

The matrix representing a linear mapping $A : \mathbb{R}^d \to \mathbb{R}^d$ in the basis $\mathcal{E}$ is computed as

$$[A]_{\mathcal{E}} := \left([A(e^{(1)})]_{\mathcal{E}}, \ldots, [A(e^{(d)})]_{\mathcal{E}} \right)$$



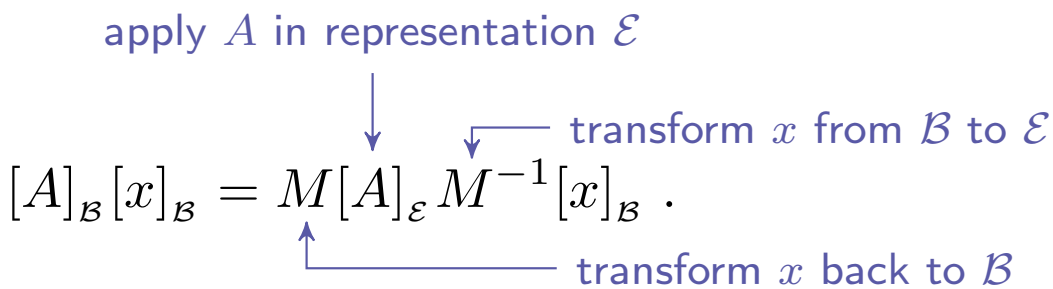
Basis Change for Linear Mappings

Transforming matrices

The matrix representing a linear mapping also changes when we change bases:

$$[A]_{\mathcal{B}} = M[A]_{\mathcal{E}} M^{-1} \ .$$

Applied to a vector x, this means:



Transforming between ONBs

If $\mathcal{V} = \{v_1, \ldots, v_m\}$ and $\mathcal{W} = \{w_1, \ldots, w_m\}$ are any two ONBs, there is an orthogonal matrix O such that

$$[A]_{\mathcal{V}} = O[A]_{\mathcal{W}} O^{-1}$$

for any linear mapping A.

Eigenvalues

We consider a square matrix $A \in \mathbb{R}^{m \times m}$.

Definition

A vector $\xi \in \mathbb{R}^m$ is called an **eigenvector** of A if the direction of ξ does not change under application of A. In other words, if there is a scalar λ such that

$$A\xi = \lambda\xi \ .$$

λ is called an **eigenvalue** of A for the eigenvector ξ.

Properties in general

- In general, eigenvalues are complex numbers $\lambda \in \mathbb{C}$.
- The class of matrices with the nicest eigen-structure are symmetric matrices, for which all eigenvectors are mutually orthogonal.

Eigenstructure of symmetric matrices

If a matrix is symmetric:

- There are rank(A) distinct eigendirections.
- The eigenvectors are pair-wise orthogonal.
- If rank$(A) = m$, there is an ONB of $\mathbb{R}^m$ consisting of eigenvectors of A.

Definiteness

type	if ...
positive definite	all eigenvalues > 0
positive semi-definite	all eigenvalues ≥ 0
negative semi-definite	all eigenvalues ≤ 0
negative definite	all eigenvalues < 0
indefinite	none of the above

Orthonormal Bases

Recall: ONB

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Transforming between ONBs

If $\mathcal{V} = \{v_1, \ldots, v_m\}$ and $\mathcal{W} = \{w_1, \ldots, w_m\}$ are ONBs, there is an orthogonal matrix O such that

$$A_{[\mathcal{V}]} = O A_{[\mathcal{W}]} O^{-1}$$

for any matrix A. By $A_{[\mathcal{V}]}$, we denote the representation of A in $\mathcal{V}$.

Eigenvector ONB

Setting

- Suppose A symmetric, $\xi_1, \ldots, \xi_m$ are eigenvectors and form an ONB.
- $\lambda_1, \ldots, \lambda_m$ are the corresponding eigenvalues.

How does A act on a vector $v \in \mathbb{R}^m$?

1. Represent v in basis $\xi_1, \ldots, \xi_m$:

$$v = \sum_{j=1}^{m} v_j^{\mathsf{A}} \xi_j \qquad \text{where } v_j^{\mathsf{A}} \in \mathbb{R}$$

2. Multiply by A: Eigenvector definition (recall: $A\xi_j = \lambda\xi_j$) yields

$$Av \quad = \quad A\Big(\sum_{j=1}^{m} v_j^{\mathsf{A}} \xi_j\Big) \quad = \quad \sum_{j=1}^{m} v_j^{\mathsf{A}} A\xi_j \quad = \quad \sum_{j=1}^{m} v_j^{\mathsf{A}} \lambda_j \xi_j$$

Conclusion

A symmetric matrix acts by scaling the directions ξ_j.

Illustration

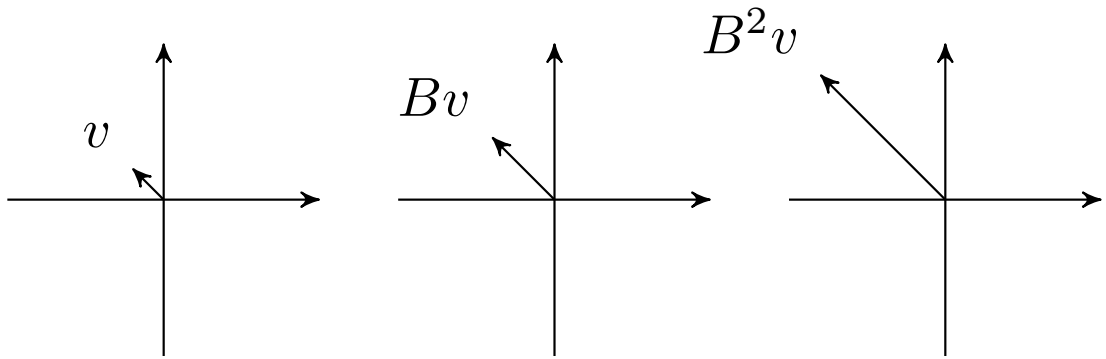
Setting

We *repeatedly* apply a symmetric matrix B to some vector $v \in \mathbb{R}^m$, i.e. we compute

$$Bv, \quad B(Bv) = B^2v, \quad B(B(Bv))) = B^3v, \quad \dots$$

How does v change?

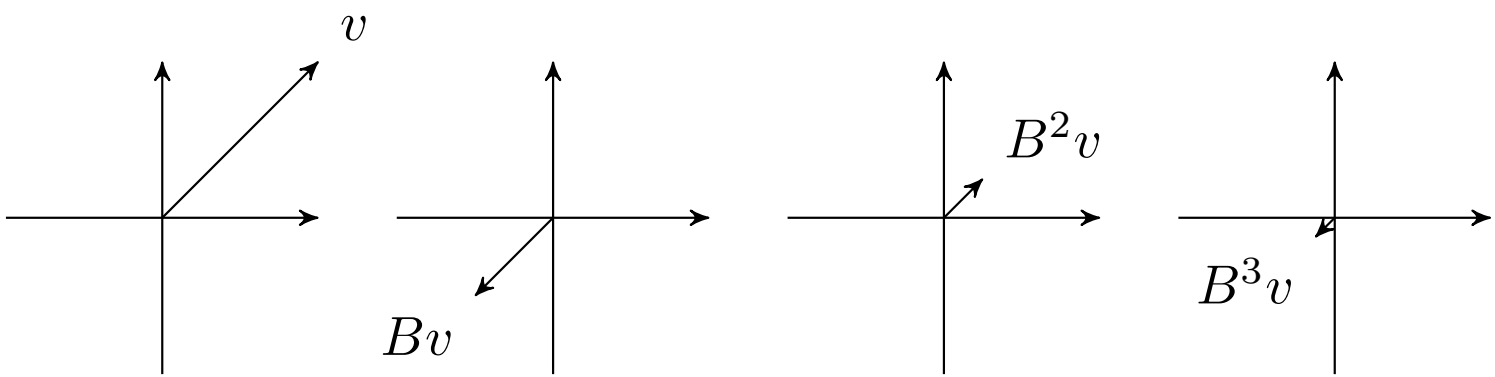
Example 1: v is an eigenvector with eigenvalue 2



The direction of v does not change, but its length doubles with each application of B.

Illustration

Example 2: v is an eigenvector with eigenvalue $-\frac{1}{2}$



For an arbitrary vector v

$$B^n v = \sum_{j=1}^{m} v_j \mathsf{B} \lambda_j^n \xi_j$$

- The weight λ_j^n grows most rapidly for eigenvalue with largest absolute value.
- Consequence:
  The direction of $B^n v$ converges to the direction of the eigenvector with largest eigenvalue as n grows large.

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