Introduction to Probabilistic Machine Learning

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Linear Basis Function Models

Overview

1. Linear Basis Function Models
2. Modelling Data
   - Modelling Text
   - Modelling Images
3. Linear Algebra
   - Vector Spaces
   - Linear Mappings and Matrices
   - Matrix Derivatives
4. Maximum A Posterior Learning and (Regularized) Least Squares

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Linear Basis Function Models

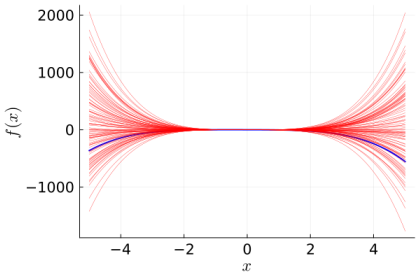
- **Linear Basis Function Models**. *Given an input space $\mathcal{X}$ and D* basis functions $\phi_j: \mathcal{X} \to \mathbb{R}$, *a* linear basis function model *is a function of the form*

$$f(x; \boldsymbol{w}) = w_0 + w_1 \cdot \phi_1(x) + w_2 \cdot \phi_2(x) + \cdots + w_D \cdot \phi_D(x)$$

- It's called a linear model, but the linearity is w.r.t. $\boldsymbol{w}$ not $x \in \mathcal{X}$!
- **Examples**: 4 basis function ($D = 4$) and 100 random parameters $\boldsymbol{w}$.

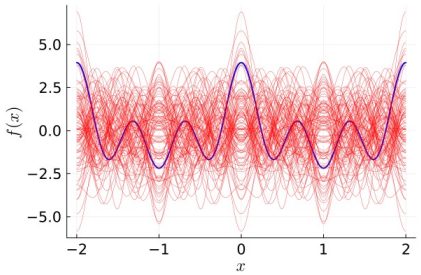
Polynomial Basis

$$\phi_j(x) = x^j$$



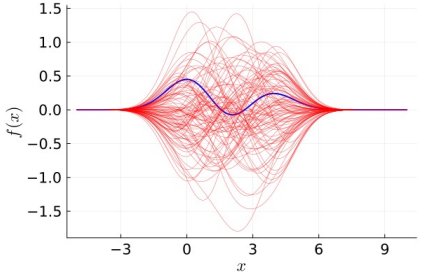
Fourier Basis

$$\phi_j(x) = \cos(\pi j \cdot x)$$



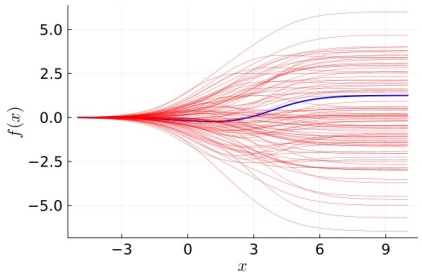
Gaussian Basis

$$\phi_j(x) = \mathcal{N}(x; j, 1)$$



Sigmoid Basis

$$\phi_j(x) = \frac{\exp(x - j)}{1 + \exp(x - j)}$$



Maximum Likelihood and Least Squares

- **Gaussian Likelihood Model**. Let's assume that our observations y are obtained from adding zero-mean normally distributed noise to $f(x; \boldsymbol{w})$

$$p(y|x, \boldsymbol{w}) = \mathcal{N}(y; f(x; \boldsymbol{w}), \sigma^2)$$

- **Maximum Likelihood Problem**. Noting that $\log(\cdot)$ is a strictly monotonic function, we see that

$$\boldsymbol{w}_{\mathrm{ML}} \coloneqq \mathrm{argmax}_{\boldsymbol{w}} \prod_i p(y_i|x_i, \boldsymbol{w}) = \mathrm{argmax}_{\boldsymbol{w}} \sum_i \log\left(\mathcal{N}(y_i|f(x_i; \boldsymbol{w}), \sigma^2)\right)$$

  - Product and sum have the same maximum, but the objective function is numerically **much** more stable as a sum of logarithms of densities (why?)

- **Least Squares**. *The minimizer of the objective function* $\sum_i \left(y_i - f(x_i; \boldsymbol{w})\right)^2$ *is* $\boldsymbol{w}_{\mathrm{ML}}$.
- **Proof**. Looking at the normal density for a given (x_i, y_i) we see that

$$\log\left(\frac{1}{\sqrt{2\pi}\sigma}\exp\left(-\frac{\left(y_i - f(x_i; \boldsymbol{w})\right)^2}{2\sigma^2}\right)\right) = \log\left(\frac{1}{\sqrt{2\pi}\sigma}\right) - \frac{1}{2\sigma^2} \cdot \underbrace{\left(y_i - f(x_i; \boldsymbol{w})\right)^2}_{\text{only part dependent on } \boldsymbol{w}}$$

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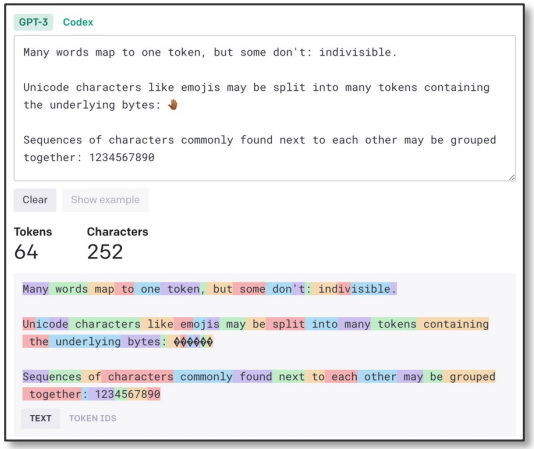
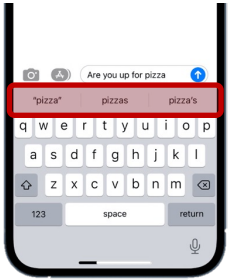
Modelling Text

- Text can be modelled at three levels of granularity:
  1. **Letters** ($\approx 10^2$ different letters in most alphabets)
  2. **Tokens** (10^3 to 10^4 different tokens in most alphabets)
  3. **Words** (10^5 to 10^6 different words in most languages)
- Modelling level of granularity depends on the application
  1. **Letters**: Compression algorithms for textual data
  2. **Tokens**: Sequence prediction for question-answering
  3. **Words**: Auto-correct function in smart keyboards





One-Hot Encoding

- Text is a sequence of text elements $s_1, s_2, s_3, \ldots$
- We often want to know the importance of each text element s_i to the target
  - **Example.** "This product shipped fast but was disappointing" has negative sentiment

s_1 s_2 s_3 s_4 s_5 s_6 s_7

Text element that is likely the expression of bad sentiment

- **One-Hot Encoding**. *Given a dictionary S and a text element $s \in S$, a one-hot encoding $\boldsymbol{\phi}_{\text{OHE}}(s)$ is an $|S|$-dimensional unit vector indexed by the elements of S that consists of 0s in all dimensions with the exception of a single 1 in the dimension indexed by s.*
  - **Example (ctd)**. If we assume the indices are $s_1, s_2, \ldots, s_7$ then

$$\boldsymbol{\phi}_{\text{OHE}}(\text{"fast"}) = \begin{bmatrix} 0 \leftarrow \text{This} \\ 0 \leftarrow \text{product} \\ 0 \leftarrow \text{shipped} \\ 1 \leftarrow \text{fast} \\ 0 \leftarrow \text{but} \\ 0 \leftarrow \text{was} \\ 0 \leftarrow \text{disappointing} \end{bmatrix}$$

- A linear model captures the *effect* of presence of a text element!

Efficient One-Hot Encoding

- In practice, the feature vector for one-hot encoded data is *never* explicitly computed because

$$\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}_{\mathrm{OHE}}(s) = \sum_{i=1}^{|S|} w_i \cdot \phi_i(s) = w_{\mathrm{idx}(s)}$$

$\mathcal{O}(|S|)$

$\mathcal{O}(\log_2|S|)$

- All we need is the inverse function mapping of an actual text element s

$$\mathrm{idx}(s) \coloneqq i \quad \Leftrightarrow \quad \phi_{\mathrm{OHE},i}(s) = 1$$

- Two common techniques for encoding a whole text
  - **Variable-length text** $s_1 s_2 \cdots$: Sum of all one-hot encoded vectors ("bag of words")

$$\boldsymbol{\phi}_{\mathrm{BOW}}(s_1 s_2 \cdots) = \sum_j \boldsymbol{\phi}_{\mathrm{OHE}}(s_j)$$

  - **Fixed-length text** $s_1 s_2 \cdots s_n$: A stacked $n \cdot |S|$ dimensional vector

$$\boldsymbol{\phi}_{\mathrm{FL}}(s_1 s_2 \cdots s_n) = \begin{bmatrix} \boldsymbol{\phi}_{\mathrm{OHE}}(s_1) \\ \vdots \\ \boldsymbol{\phi}_{\mathrm{OHE}}(s_n) \end{bmatrix}$$

$\mathcal{O}(n \cdot \log_2|S|)$

Bag of words **cannot** learn "positional" effect of text elements

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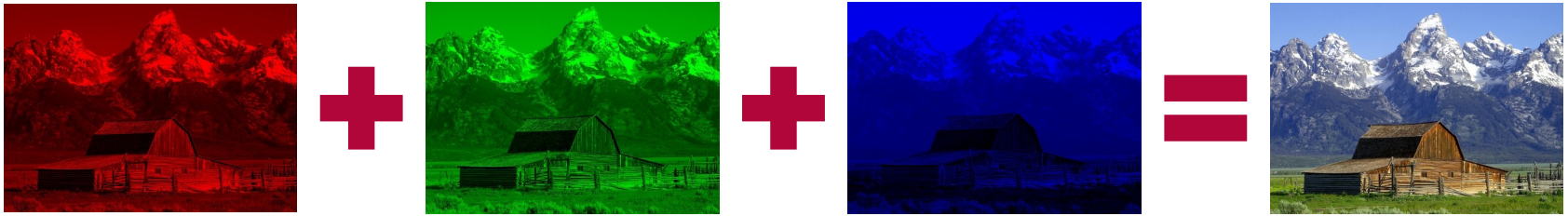
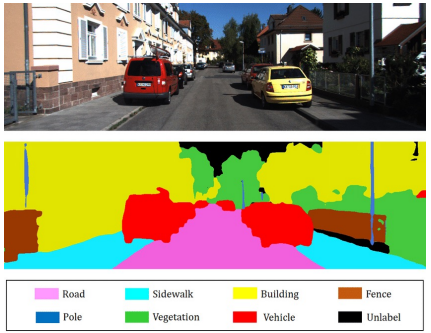
Modelling Images

- **Raw image data**. *An image is a rectangular array of picture elements (“pixels”) that consist of a triple of intensities of the base colors red, blue and green.*



- Images can also be modelled at three levels of granularity depending on application
  1. **Pixels**: Image segmentation
  2. (Non-overlapping) **patches**: Object recognition
  3. **Whole image**: Image classification



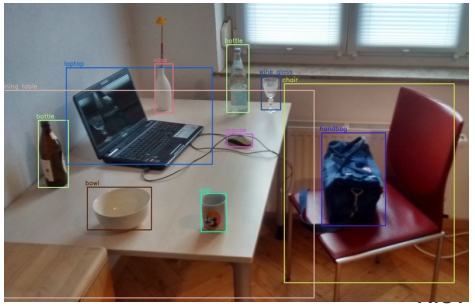


Image Content in Frequency and Location

- Image data contains signal (photon counts) at *fixed* locations in the image

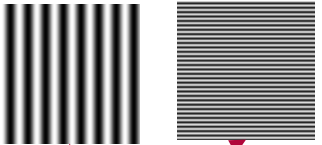
$$\boldsymbol{\phi}_{\text{RGB}}\left(\text{  }\right) = \begin{bmatrix} 127 \\ 0 \\ \vdots \\ 32 \\ 6 \end{bmatrix}$$

- 127 ← Red value at location (1,1)
- 0 ← Green value at location (1,1)
- 32 ← Green value at location (800,600)
- 6 ← Blue value at location (800,600)

- **Observation**. Recurring patterns are more visible in the frequency domain.
- **Idea**. Discrete Fourier transform (DFT) to transform the image

$$\boldsymbol{\phi}_{\text{DFT}}(x) = \boldsymbol{F}_{\text{DFT}}\boldsymbol{\phi}_{\text{RGB}}(x)$$

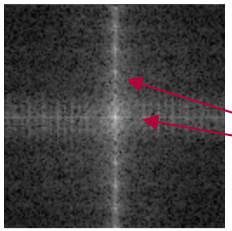
  - In practice, there is a $\mathcal{O}(\#\text{pixel} \cdot \log(\#\text{pixel}))$ algorithm for fast Fourier transform (FFT)



$$\boldsymbol{F}_{\text{DFT}} = \boldsymbol{W}_{\text{DFT}} \otimes \boldsymbol{W}_{\text{DFT}}$$

Kronecker product of 1D discrete Fourier transform $\boldsymbol{W}_{\text{DFT}}$

Raw image (in single-grey channel)

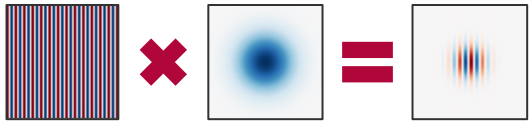


Fourier transform of image

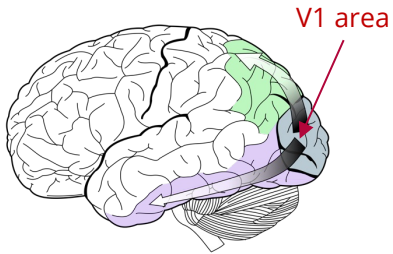
Horizontal and vertical patterns by single features

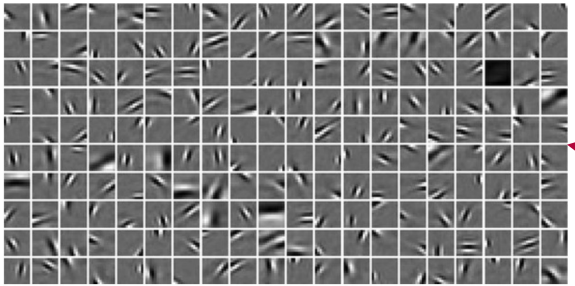
Gabor Wavelets: Mixing Location and Frequency

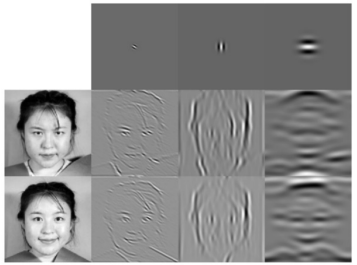
- Both representations are extremes:
  - **Raw image**: Single features $\phi_{\mathrm{RGB},i}(x)$ at a location without frequency
  - **DFT image**: Single features $\phi_{\mathrm{DFT},i}(x)$ in frequency without a location
- **Gabor wavelets**. A *Gabor wavelet* is a set of basis functions that is obtained by multiplying a Fourier basis function with a Gaussian density.



  - Combine both spatial and frequency information in image features
  - Basis functions for sparse encoding by the brain in V1







Dennis Gabor
(1900 – 1978)

Filters "implemented" in the V1 (sparse coding!)

Bruno Olshausen & David Field (1997). Sparse Coding with Overcomplete Basis Set: A Strategy Employed by V1?

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Vector Spaces

- **Vector Space**. *A vector space is a set V that satisfies the following axioms: There exists a null element $\mathbf{0} \in V$ such that for all $\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w} \in V$ and scalars $a, b \in \mathbb{R}$*
  1. **Associativity**: $\boldsymbol{u} + (\boldsymbol{v} + \boldsymbol{w}) = (\boldsymbol{u} + \boldsymbol{v}) + \boldsymbol{w}$
  2. **Commutativity**: $\boldsymbol{u} + \boldsymbol{v} = \boldsymbol{v} + \boldsymbol{u}$
  3. **Identity element (of vector addition)**: $\boldsymbol{v} + \mathbf{0} = \boldsymbol{v}$
  4. **Inverse element**: $\boldsymbol{v} + (-\boldsymbol{v}) = \mathbf{0}$
  5. **Identity element (of scalar multiplication)**: $1 \cdot \boldsymbol{v} = \boldsymbol{v}$
  6. **Distributivity (w.r.t. vector addition)**: $a \cdot (\boldsymbol{u} + \boldsymbol{v}) = a \cdot \boldsymbol{u} + a \cdot \boldsymbol{v}$
  7. **Distributivity (w.r.t. scalar addition)**: $(a + b) \cdot \boldsymbol{v} = a \cdot \boldsymbol{v} + b \cdot \boldsymbol{v}$
- **Two Examples**
  - **Points in space**: $V = \mathbb{R}^d$ with $\begin{pmatrix} u_1 \\ \vdots \\ u_d \end{pmatrix} + \begin{pmatrix} v_1 \\ \vdots \\ v_d \end{pmatrix} = \begin{pmatrix} u_1 + v_1 \\ \vdots \\ u_d + v_d \end{pmatrix}$ and $a \cdot \begin{pmatrix} u_1 \\ \vdots \\ u_d \end{pmatrix} = \begin{pmatrix} au_1 \\ \vdots \\ au_d \end{pmatrix}$
  - **Functions on** $\mathbb{R}$: $V = \mathbb{R}^{\mathbb{R}}$ with $f + g = x \mapsto f(x) + g(x)$ and $a \cdot f = x \mapsto a \cdot f(x)$

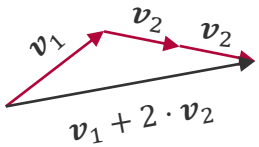
Bernhard Bolzano
(1781 – 1848)

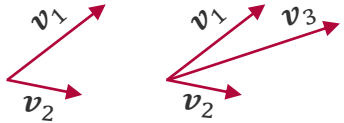
Linear Independence, Span and Basis

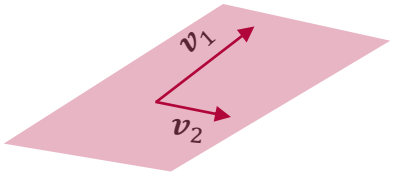
- **Linear combination**. *Given a set $\boldsymbol{v}_1, \boldsymbol{v}_2, \dots, \boldsymbol{v}_n$ of a vector space V, a* linear combination *is defined by ($a_1, a_2, \dots, a_n$ are called coefficients)*

$$a_1 \cdot \boldsymbol{v}_1 + a_2 \cdot \boldsymbol{v}_2 + \cdots + a_n \cdot \boldsymbol{v}_n$$

- **Linear independence**. *A set $\boldsymbol{v}_1, \boldsymbol{v}_2, \dots, \boldsymbol{v}_n$ is called* linearly independent *if no $\boldsymbol{v}_i$* can be written as a linear combination of $\boldsymbol{v}_1, \dots, \boldsymbol{v}_{i-1}, \boldsymbol{v}_{i+1}, \dots, \boldsymbol{v}_n$.
- **Span**. *Given a set $\boldsymbol{v}_1, \boldsymbol{v}_2, \dots, \boldsymbol{v}_n$ of a vector space V, the* span $\text{span}(\boldsymbol{v}_1, \boldsymbol{v}_2, \dots, \boldsymbol{v}_n)$ *is the set of all* linear combinations of $\boldsymbol{v}_1, \boldsymbol{v}_2, \dots, \boldsymbol{v}_n$.
  - **Example**:
    - $\text{span}(\boldsymbol{v}_1)$ is the line through the origin along $\boldsymbol{v}_1$
    - $\text{span}(\boldsymbol{v}_1, \boldsymbol{v}_2)$ is the plane through the origin along $\boldsymbol{v}_1$ and $\boldsymbol{v}_2$
- **Basis**. *A subset $\boldsymbol{b}_1, \boldsymbol{b}_2, \dots, \boldsymbol{b}_n$ of a vector space V is called a* basis *if its span equals the whole vector space, that is, $span(\boldsymbol{b}_1, \boldsymbol{b}_2, \dots, \boldsymbol{b}_n) = V$.*
- **Dimensionality**. *All bases of a vector space V have the same cardinality called the* dimensionality *of the vector space,* $\dim(V)$.

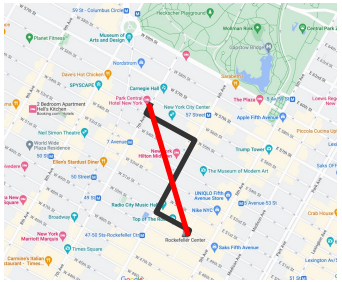






Scalar Products and Inner Product Spaces

- So far, a vector space is a set but there is no notion of **distance**!
  - In New York, the **walking distance** between two points is much longer than the **flying distance**!



- **Metric space**. *A metric space is a vector space V together with a metric $d: V \times V \to \mathbb{R}^+$ that has the following properties for all $\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z}$:*

$$d(\boldsymbol{x}, \boldsymbol{y}) = 0 \Leftrightarrow \boldsymbol{x} = \boldsymbol{y}$$

$$d(\boldsymbol{x}, \boldsymbol{y}) = d(\boldsymbol{y}, \boldsymbol{x}) \quad \leftarrow \text{symmetry}$$

$$d(\boldsymbol{x}, \boldsymbol{y}) \leq d(\boldsymbol{x}, \boldsymbol{z}) + d(\boldsymbol{z}, \boldsymbol{y}) \quad \leftarrow \text{triangle inequality}$$

- **Inner product space**. *An inner product space is a vector space together with an inner product function $\langle \cdot, \cdot \rangle: V \times V \to \mathbb{R}^+$ that has the following properties for all $\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z}$:*

$$\langle \boldsymbol{x}, \boldsymbol{x} \rangle = 0 \Leftrightarrow \boldsymbol{x} = \boldsymbol{0}$$

$$\langle \boldsymbol{x}, \boldsymbol{y} \rangle = \langle \boldsymbol{y}, \boldsymbol{x} \rangle \quad \leftarrow \text{symmetry}$$

$$\langle a \cdot \boldsymbol{x} + b \cdot \boldsymbol{y}, \boldsymbol{z} \rangle = a\langle \boldsymbol{x}, \boldsymbol{z} \rangle + b\langle \boldsymbol{y}, \boldsymbol{z} \rangle \quad \leftarrow \text{linearity}$$

- *Every inner product space is a metric space with $d(\boldsymbol{x}, \boldsymbol{y}) = \|\boldsymbol{x} - \boldsymbol{y}\| = \sqrt{\langle \boldsymbol{x} - \boldsymbol{y}, \boldsymbol{x} - \boldsymbol{y} \rangle}$!*

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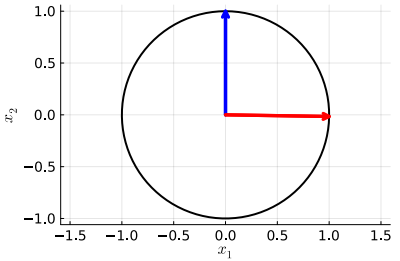
Linear Mappings and Matrices

- **Linear mapping**. *A function $f: V \to W$ is a* linear mapping *between vector space V and W if for any two vectors $\boldsymbol{u}, \boldsymbol{v} \in V$ and any scalar $c \in \mathbb{R}$:*

$$f(\boldsymbol{u} + \boldsymbol{v}) = f(\boldsymbol{u}) + f(\boldsymbol{v})$$
$$f(c \cdot \boldsymbol{u}) = c \cdot f(\boldsymbol{u})$$

  - Addition and scalar multiplication can be applied before or after the map!
  - It follows that $f(\mathbf{0}) = f(0 \cdot \boldsymbol{v}) = 0 \cdot f(\boldsymbol{v}) = \mathbf{0}$!



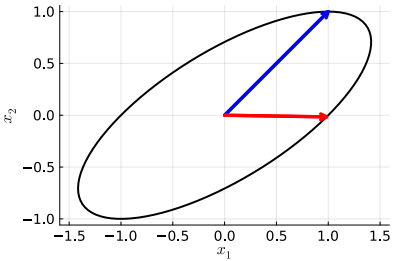
$$f(\boldsymbol{x}) = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix} \boldsymbol{x}$$

- **Theorem**. *Every linear mapping $f: V \to W$ between V and W of dimension n and m can be represented via a matrix multiplication with an $m \times n$ matrix $\boldsymbol{A}$. The rank of $\boldsymbol{A}$ is the dimensionality of the image of W, that is* $\operatorname{rank}(\boldsymbol{A}) = \dim(W)$.
  - **Proof**. If $\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_n\}$ is a basis for V and $\{\boldsymbol{w}_1, \ldots, \boldsymbol{w}_m\}$ is a basis for W then we know

$$f(\boldsymbol{v}_j) = a_{1j} \cdot \boldsymbol{w}_1 + \cdots + a_{mj} \cdot \boldsymbol{w}_m$$

$$f(\boldsymbol{v}) = f(c_1 \boldsymbol{v}_1 + \cdots + c_n \boldsymbol{v}_n) = c_1 \cdot f(\boldsymbol{v}_1) + \cdots + c_n \cdot f(\boldsymbol{v}_n) = \sum_{i=1}^{m} [\boldsymbol{A}\boldsymbol{c}]_j \cdot \boldsymbol{w}_j$$

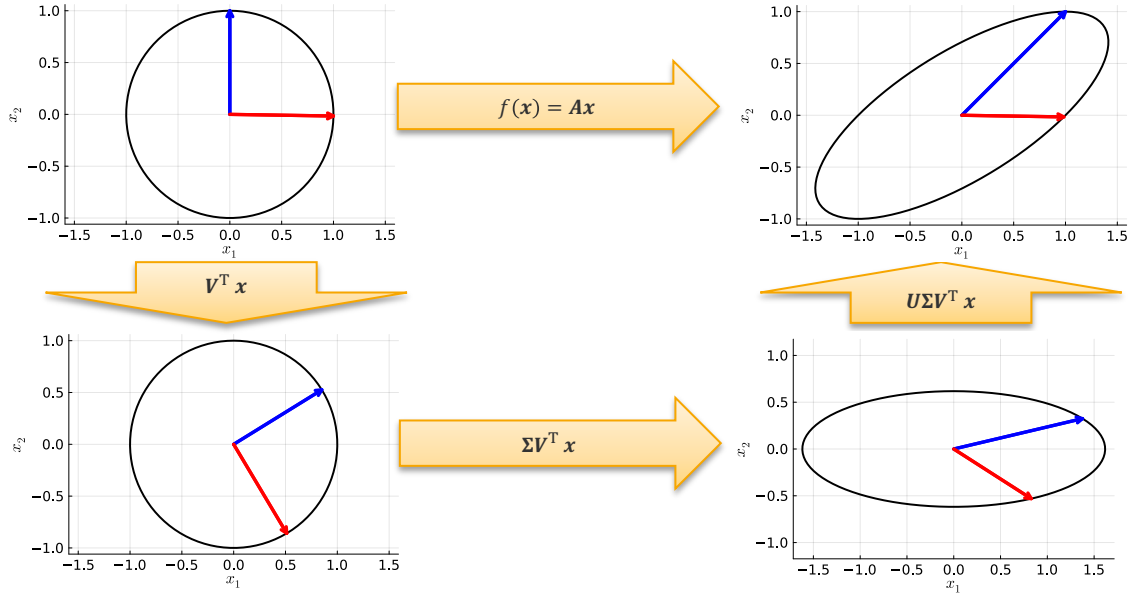
  - For $V = \mathbb{R}^n$ and $W = \mathbb{R}^m$, the columns of $\boldsymbol{A}$ are the images of the basis vectors in $\mathbb{R}^n$.
  - For any matrix $\boldsymbol{A} \in \mathbb{R}^{n \times m}$, $\operatorname{rank}(A) \leq \min(n, m)$.



Singular Value Decomposition

- **Singular Value Decomposition**. *Any matrix $\boldsymbol{A} \in \mathbb{R}^{n \times m}$ has a decomposition into three matrices $\boldsymbol{U} \in \mathbb{R}^{n \times n}$, $\boldsymbol{\Sigma} \in \mathbb{R}^{n \times m}$ and $\boldsymbol{V} \in \mathbb{R}^{m \times m}$ such that $\boldsymbol{U}\boldsymbol{U}^{\mathrm{T}}$ and $\boldsymbol{V}\boldsymbol{V}^{\mathrm{T}}$ are the identity and $\boldsymbol{\Sigma}$ is only non-zero on diagonal elements*

$$\boldsymbol{A} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^{\mathrm{T}}$$



Matrix Types and Properties

- **Square Matrix**. *A matrix $\boldsymbol{A} \in \mathbb{R}^{n \times m}$ where $m = n$ is called a* square matrix*. It parameterizes mappings of a space onto itself.*
- **Symmetric Matrix**. *A square matrix $\boldsymbol{A}$ is called* symmetric *if and only if $\boldsymbol{A} = \boldsymbol{A}^{\mathrm{T}}$.*
  - $\boldsymbol{A} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^{\mathrm{T}} = \left(\boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^{\mathrm{T}}\right)^{\mathrm{T}} = \boldsymbol{V}\boldsymbol{\Sigma}\boldsymbol{U}^{\mathrm{T}}$ implies that $\boldsymbol{V} = \boldsymbol{U}$ if all singular values are non-zero.
- **Diagonal Matrix**. *A square matrix $\boldsymbol{A}$ is called* diagional *if $\boldsymbol{A}_{ij} = 0$ for all $i \neq j$.*
  - Geometrically, a diagional matrix is an axis scaling (mapping).
  - A special diagional matrix is $\mathbf{A}_{ii} = 1$ which is also called identity matrix.
- **Orthogonal Matrix**. *A square matrix $\boldsymbol{A}$ is called orthogonal if $\boldsymbol{A}\boldsymbol{A}^{\mathrm{T}} = \boldsymbol{I}$.*
  - Geometrically, an orthogonal matrix is a rotation and mirroring (mapping).
- **Positive semi-definite matrix**. *A symmetric matrix $\boldsymbol{A}$ is called* positive definite *if and only if*

$$\forall \boldsymbol{x} \neq \mathbf{0} : \boldsymbol{x}^{\mathrm{T}}\boldsymbol{A}\boldsymbol{x} > 0$$

  - If $\boldsymbol{x} = \boldsymbol{U}\boldsymbol{y}$ then $\boldsymbol{x}^{\mathrm{T}}\boldsymbol{A}\boldsymbol{x} = \boldsymbol{y}^{\mathrm{T}}\boldsymbol{U}^{\mathrm{T}}\boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{U}\boldsymbol{U}^{\mathrm{T}}\boldsymbol{y} = \sum_i \sigma_i \, y_i^2 > 0$. Hence, positive definiteness means that all singular values are strictly positive, that is, no axis is inverted or removed.

Determinant of a Matrix

- **Determinant**. *The determinant,$|\boldsymbol{A}|$, of a square matrix $\boldsymbol{A} \in \mathbb{R}^{n \times n}$ is the unique function that has the following three properties for any $c \in \mathbb{R}$:*

$$|\boldsymbol{I}| = 1$$
$$\left|[\boldsymbol{a}_1, \dots, \boldsymbol{a}_i, \dots, \boldsymbol{a}_j, \dots, \boldsymbol{a}_n]\right| = -\left|[\boldsymbol{a}_1, \dots, \boldsymbol{a}_j, \dots, \boldsymbol{a}_i, \dots, \boldsymbol{a}_n]\right|$$
$$|[\boldsymbol{a}_1, \dots, c \cdot \boldsymbol{u} + \boldsymbol{v}, \dots, \boldsymbol{a}_n]| = c \cdot |[\boldsymbol{a}_1, \dots, \boldsymbol{u}, \dots, \boldsymbol{a}_n]| + |[\boldsymbol{a}_1, \dots, \boldsymbol{v}, \dots, \boldsymbol{a}_n]|$$

Pierre-Simon Laplace (1749 – 1827)

- **Laplace Expansion**. *If $\boldsymbol{A}_{[i,j]}$ is obtained from $\boldsymbol{A}$ by removing row i and column j*

$$\forall i: \quad |\boldsymbol{A}| = \sum_{j=1}^{n} (-1)^{i+j} \boldsymbol{A}_{i,j} \cdot \left|\boldsymbol{A}_{[i,j]}\right|$$

  - Not useful for computation as $O(n!)$ but useful for proofs!
  - **Properties**: The determinant has the following two properties

$$|\boldsymbol{AB}| = |\boldsymbol{A}| \cdot |\boldsymbol{B}|$$
$$\left|\boldsymbol{A}^{\mathrm{T}}\right| = |\boldsymbol{A}|$$

Note that this implies for orthogonal matrices $\boldsymbol{U}$ that
$1 = |\boldsymbol{I}| = \left|\boldsymbol{U}\boldsymbol{U}^{\mathrm{T}}\right| = |\boldsymbol{U}| \cdot \left|\boldsymbol{U}^{\mathrm{T}}\right| = |\boldsymbol{U}|^2 \Leftrightarrow |\boldsymbol{U}| = \pm 1$

- **Theorem**: *The determinant $|\boldsymbol{A}|$ of a matrix $\boldsymbol{A}$ is the product of all singular values.*
  - **Proof**. $|\boldsymbol{A}| = \left|\boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^{\mathrm{T}}\right| = |\boldsymbol{U}| \cdot |\boldsymbol{\Sigma}| \cdot \left|\boldsymbol{V}^{\mathrm{T}}\right| = |\boldsymbol{\Sigma}| = \prod_i \sigma_i$
  - **Corollary**. The determinant a is the volume of the parallelepiped of the new basis!

Generalized Inverse of a Matrix

- **Inverse**. *The inverse $\boldsymbol{A}^{-1}$ of a full-rank square matrix $\boldsymbol{A}$ has the property that*
$$\boldsymbol{A}^{-1}\boldsymbol{A} = \boldsymbol{A}\boldsymbol{A}^{-1} = \boldsymbol{I}$$
- **Pseudo-Inverse (Moore-Penrose)**. *For any matrix $\boldsymbol{A} \in \mathbb{R}^{n\times m}$, the pseudo-inverse $\boldsymbol{A}^{+} \in \mathbb{R}^{m\times n}$ has the following properties (it is identical to $\boldsymbol{A}^{-1}$ when $\boldsymbol{A}$ is a full-rank and square matrix)*
$$\boldsymbol{A}\boldsymbol{A}^{+}\boldsymbol{A} = \boldsymbol{A} \; and \; \boldsymbol{A}^{+}\boldsymbol{A}\boldsymbol{A}^{+} = \boldsymbol{A}^{+}$$
$$(\boldsymbol{A}\boldsymbol{A}^{+})^{\mathrm{T}} = \boldsymbol{A}\boldsymbol{A}^{+} \; and \; (\boldsymbol{A}^{+}\boldsymbol{A})^{\mathrm{T}} = \boldsymbol{A}^{+}\boldsymbol{A}$$
- **Pseudo-Inverse Computation**. If a matrix either has full column or row rank
  - If $\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}$ exists, then $\boldsymbol{A}^{+} = \left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\boldsymbol{A}^{\mathrm{T}}$
  - If $\left(\boldsymbol{A}\boldsymbol{A}^{\mathrm{T}}\right)^{-1}$ exists, then $\boldsymbol{A}^{+} = \boldsymbol{A}^{\mathrm{T}}\left(\boldsymbol{A}\boldsymbol{A}^{\mathrm{T}}\right)^{-1}$
- **Least Squares Property**. *For any matrix $\boldsymbol{A}$ and vector $\boldsymbol{b}$, the minimizer of the least-squares difference between $\boldsymbol{A}\boldsymbol{x}$ and $\boldsymbol{b}$ is given by $\boldsymbol{A}^{+}\boldsymbol{b}$. In other words, for all $\boldsymbol{x}$*
$$\|\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b}\|^2 \geq \|\boldsymbol{A}\boldsymbol{A}^{+}\boldsymbol{b} - \boldsymbol{b}\|^2$$

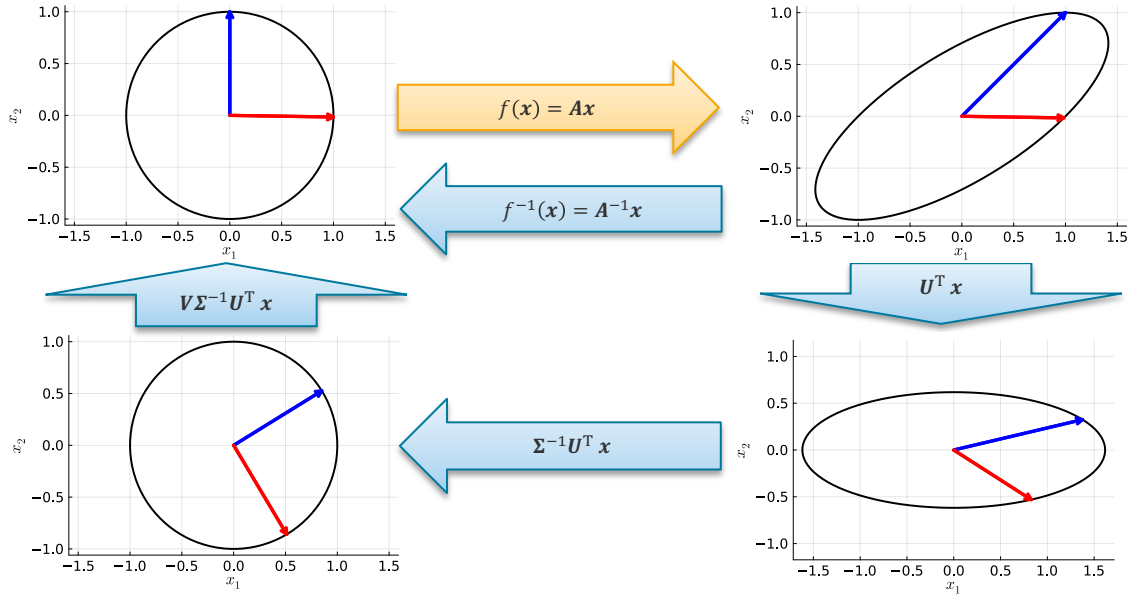
Eliakim Hastings Moore
(1862 – 1932)

Sir Roger Penrose
(1931 –)

Generalized Inverse of a Matrix (SVD)

- But what if neither row or column rank are full?
  - Then we can use the singular value decomposition $\boldsymbol{A} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^{\mathrm{T}}$ because

$$\boldsymbol{A}^{+} = \boldsymbol{V}\boldsymbol{\Sigma}^{-1}\boldsymbol{U}^{\mathrm{T}}$$



Maximum Likelihood Revisited

- **Maximum Likelihood Problem (in matrix notation).** If $\boldsymbol{\Phi}_{ij} = \phi_j(x_i)$

$$\boldsymbol{w}_{\mathrm{ML}} \coloneqq \mathrm{argmin}_{\boldsymbol{w}} \|\boldsymbol{\Phi}\boldsymbol{w} - \boldsymbol{y}\|^2$$

  - If we have more data points $x_1, \ldots, x_N$ than basis functions $\phi_1, \ldots, \phi_D$, then $\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi}$ has full rank and the minimizer can be computed from the Moore-Penrose inverse

$$\boldsymbol{w}_{\mathrm{ML}} = \left(\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi}\right)^{-1}\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{y}$$

- **Computational complexity**: $O(ND^2)$
  1. The matrix multiplication $\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi}$ is an $O(ND^2)$ operation
  2. The inverse $\left(\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi}\right)^{-1}$ is an $O(D^3)$ operation
  3. The matrix product $\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{y}$ is an $O(ND)$ operation
  4. The matrix product $\left[\left(\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi}\right)^{-1}\right] \cdot [\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{y}]$ is an $O(D^2)$ operation
- **Projection**. *The matrix $\boldsymbol{P} \coloneqq \boldsymbol{\Phi}(\boldsymbol{\Phi}^T\boldsymbol{\Phi})^{-1}\boldsymbol{\Phi}^T$ is a projection mapping of a target vector $\boldsymbol{y}$ to its least-square approximation in the span of the basis functions!*
  - All projections have the property that $\boldsymbol{P}\boldsymbol{P} = \boldsymbol{P}$! (proof)

Cholesky Decomposition

- **Numerical Challenge**: Given a symmetric, positive-definite matrix $\boldsymbol{A} \in \mathbb{R}^{n \times n}$ and a vector $\boldsymbol{b} \in \mathbb{R}^n$ find the solution $\boldsymbol{x}$ such that

$$\boldsymbol{Ax} = \boldsymbol{b}$$

- **Naïve Solution**: Invert the matrix $\boldsymbol{A}$ and compute

$$\boldsymbol{x} = \boldsymbol{A}^{-1}\boldsymbol{b}$$

  - **Challenges**: If $\boldsymbol{A}$ has some singular values close to zero, this is numerically unstable!

- **Cholesky Decomposition**: Every positive-definitive matrix $\boldsymbol{A} \in \mathbb{R}^{n \times n}$ has a unique decomposition into a lower-triangular matrix $\boldsymbol{L} \in \mathbb{R}^{n \times n}$, $L_{ij} = 0$ if $j > i$

$$\boldsymbol{A} = \boldsymbol{L}\boldsymbol{L}^T$$

  - **Advantage**: Finding $\boldsymbol{y}$ such that $\boldsymbol{Ly} = \boldsymbol{b}$ can be done in $O(n^2)$ without an inverse simply using back-substitution (written as $\boldsymbol{y} = \boldsymbol{L} \backslash \boldsymbol{b}$)!

- **Cholesky Solution**: Find the solution $\boldsymbol{x}$ for $\boldsymbol{Ax} = \boldsymbol{b}$ is a two-step algorithm
  1. Compute $\boldsymbol{y} = \boldsymbol{L} \backslash \boldsymbol{b}$
  2. Compute $\boldsymbol{x} = \boldsymbol{L}^T \backslash \boldsymbol{y}$

$$\boldsymbol{Ax} = \boldsymbol{b} \Leftrightarrow \boldsymbol{L}\boldsymbol{L}^T\boldsymbol{x} = \boldsymbol{b}$$

$$\boldsymbol{Ly} = \boldsymbol{b}$$

André-Louis Cholesky
(1875 – 1918)

$$\begin{pmatrix} L_{11} & 0 & 0 \\ L_{21} & L_{22} & 0 \\ L_{31} & L_{32} & L_{33} \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} b_1 \\ b \\ b_3 \end{pmatrix}$$

$$y_1 = \frac{b_1}{L_{11}}$$

$$y_2 = \frac{b_2 - L_{21} \cdot y_1}{L_{22}}$$

$$y_3 = \frac{b_3 - L_{31} \cdot y_1 - L_{32} \cdot y_2}{L_{33}}$$

Overview

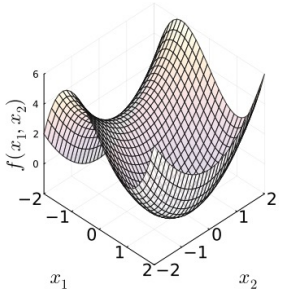
1. Linear Basis Function Models
2. Modelling Data
   - Modelling Text
   - Modelling Images
3. Linear Algebra
   - Vector Spaces
   - Linear Mappings and Matrices
   - **Matrix Derivatives**
4. Maximum A Posterior Learning and (Regularized) Least Squares

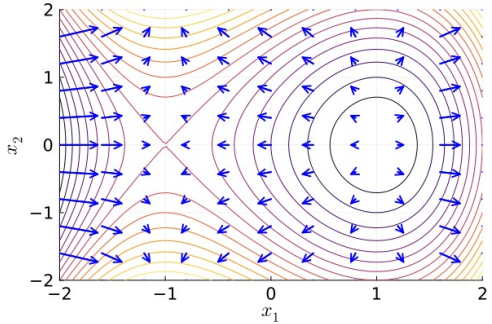
Derivates of Vector-Valued Functions

- **Derivate of vector-valued functions**. *Let* $g: \mathbb{R}^m \to \mathbb{R}^n$ *be a vector-valued function. Then the* $m \times n$ *matrix* $\frac{\partial g(\boldsymbol{x})}{\partial \boldsymbol{x}}$ *of derivates is defined by*

$$\frac{\partial g(\boldsymbol{x})}{\partial \boldsymbol{x}} := \left[\frac{\partial g_j(\boldsymbol{x})}{\partial x_i}\right]_{i,j=1}^{m,n} = \begin{bmatrix} \frac{dg_1(\boldsymbol{x})}{dx_1} & \cdots & \frac{dg_n(\boldsymbol{x})}{dx_1} \\ \vdots & \ddots & \vdots \\ \frac{dg_1(\boldsymbol{x})}{dx_m} & \cdots & \frac{dg_n(\boldsymbol{x})}{dx_m} \end{bmatrix}$$

- **Example**. Let $g(x_1, x_2) = x_1^3 - 3x_1 + x_2^2$





Derivates of Linear Mappings

- **Theorem**. *Let $f(\boldsymbol{x})$ be a linear mapping, $f(\boldsymbol{x}) = \boldsymbol{A}\boldsymbol{x} + \boldsymbol{b}$. Then*

$$\frac{\partial f(\boldsymbol{x})}{\partial \boldsymbol{x}} = \boldsymbol{A}^{\mathrm{T}}$$

- **Theorem**. *Let $f(\boldsymbol{x})$ be a quadratic form, $f(\boldsymbol{x}) = \boldsymbol{x}^{\mathrm{T}}\boldsymbol{A}\boldsymbol{x}$. Then*

$$\frac{\partial f(\boldsymbol{x})}{\partial \boldsymbol{x}} = 2\boldsymbol{A}^{\mathrm{T}}\boldsymbol{x}$$

- **Example**. Let us consider $f(\boldsymbol{x}) = \|\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b}\|^2 = (\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b})^{\mathrm{T}}(\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b})$

$$f(\boldsymbol{x}) = \boldsymbol{x}^{\mathrm{T}}\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\boldsymbol{x} - 2\boldsymbol{b}^{T}\boldsymbol{A}\boldsymbol{x} + \boldsymbol{b}^{\mathrm{T}}\boldsymbol{b}$$

$$\left.\frac{\partial f(\boldsymbol{x})}{\partial \boldsymbol{x}}\right|_{\boldsymbol{x}=\boldsymbol{x}^*} = 2\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\boldsymbol{x}^* - 2\boldsymbol{A}^{\mathrm{T}}\boldsymbol{b} = \boldsymbol{0}$$

$$\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)\boldsymbol{x}^* = \boldsymbol{A}^{\mathrm{T}}\boldsymbol{b}$$

$$\boldsymbol{x}^* = \underbrace{\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\boldsymbol{A}^{\mathrm{T}}}_{\text{Moore–Penrose Inverse}}\ \boldsymbol{b}$$

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Maximum A Posteriori Learning

- **Gaussian Likelihood Model**. Let's assume that our observations y are obtained from adding zero-mean normally distributed noise

$$p(y|x, \boldsymbol{w}) = \mathcal{N}(y; f(x; \boldsymbol{w}), \sigma^2)$$

- **Gaussian Prior Model**. Let's assume a componentwise Gaussian over $\boldsymbol{w}$

$$p(\boldsymbol{w}) = \prod_d \mathcal{N}(w_d; 0, \tau^2)$$

- **Maximum A-Posterior Problem**. Noting that $\log(\cdot)$ is strictly monotonic

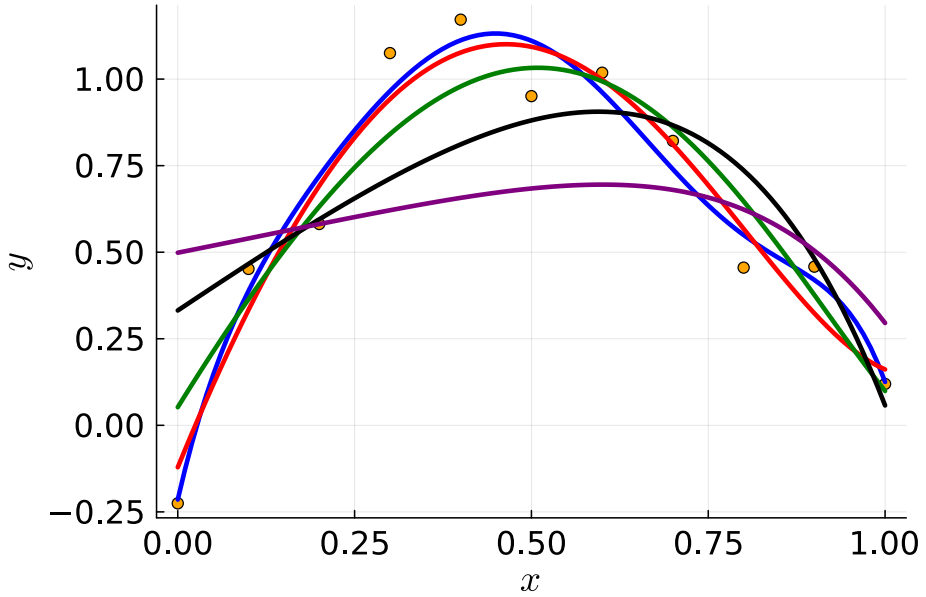
$$\boldsymbol{w}_{\text{MAP}} \coloneqq \text{argmax}_{\boldsymbol{w}} \underbrace{\prod_i p(y_i|x_i, \boldsymbol{w})}_{p(D|\boldsymbol{w})} \cdot \underbrace{\prod_d p(w_d)}_{p(\boldsymbol{w})} = \text{argmin}_{\boldsymbol{w}} \frac{1}{2\sigma^2} \|\boldsymbol{\Phi}\boldsymbol{w} - \boldsymbol{y}\|^2 + \frac{1}{2\tau^2} \boldsymbol{w}^{\mathrm{T}} \boldsymbol{w}$$

$$\left. \frac{\partial \log\big(p(D|\boldsymbol{w}) \cdot p(\boldsymbol{w})\big)}{\partial \boldsymbol{w}} \right|_{\boldsymbol{w}=\boldsymbol{w}_{\text{MAP}}} = \frac{1}{\sigma^2}\left(\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi}\boldsymbol{w}_{\text{MAP}} - \boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{y}\right) + \frac{1}{\tau^2}\boldsymbol{w}_{\text{MAP}} = \boldsymbol{0}$$

$$\boldsymbol{w}_{\text{MAP}} = \left(\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi} + \frac{\sigma^2}{\tau^2}\boldsymbol{I}\right)^{-1} \boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{y}$$

Maximum A Posteriori Learning: Polynomial Regression

$$f(x; \boldsymbol{w}) = \sum_{d=0}^{6} w_d \cdot x^d$$



$\frac{\sigma^2}{\tau^2} = 0$

$\frac{\sigma^2}{\tau^2} = 10^{-3}$

$\frac{\sigma^2}{\tau^2} = 10^{-2}$

$\frac{\sigma^2}{\tau^2} = 10^{-1}$

$\frac{\sigma^2}{\tau^2} = 10^{-0}$

Summary

- **Linear Basis Functions Models**
  - Non-linear prediction models can be formed with non-linear basis functions
  - Linearity is in the parameters, *not* the input dimensions of the data
- **Modelling Data**
  - Both textual and image data can be represented at different levels of granularity
  - Images should ideally be represented in terms of feature of location and frequency: Gabor wavelets/filters are excellent candidate functions for such features
- **Linear Mappings and Matrices**
  - All linear mappings can be expressed via matrix products
  - The singular value decomposition is the rotation-scaling-rotation view on a mapping
  - The inverse and determinant are critical for solving least-squares problems
- **Matrix Derivatives**
  - Matrix derivatives are a natural generalization of 1D-function derivatives
  - Regularized least-square has closed-form solution using matrix derivatives

See you next week!