Parametric modeling of Earth system processes

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Modeling of Earth System Data

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Parametric modeling — Overview

1. Vectors, scalar product, distances
   - Vector operations, difference vectors, distances, angles
   - Minimum distances between points and geometric objects
2. Vector algebra concepts in data analysis and modeling
   - Data vectors, mean, variance, covariance, correlation
   - Geometrical characterization of the least squares principle
   - Further example of inner (scalar) product spaces
3. Linear equations, inversion, matrix decompositions
   - Matrix multiplication, linear equations, inversion
   - Matrix decompositions using eigenvalues and singular values
4. Data modeling and numerical linear algebra
   - Parametric modeling, linear problems, design matrix
   - Condition number, generalized inverses, stability

Vectors, scalar product, distances

Vector addition and scaling

Vectors are objects in a *linear space*: one can add (and subtract) vectors in a meaningful way, and also multiply them with scalar values.

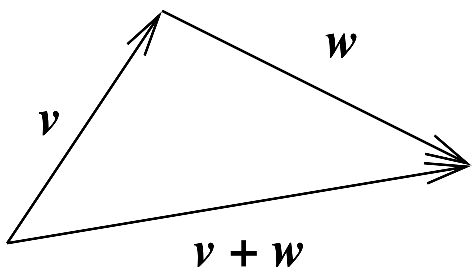
Important example: *n-tuples* (ordered lists) of real numbers.

Notation: $\boldsymbol{v}$, $\vec{v}$, $\underline{v}$.

In three dimensions ($n = 3$): $\boldsymbol{v} = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix}$, $\boldsymbol{w} = \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix}$

Addition of two vectors:

$$\begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} + \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix} = \begin{pmatrix} v_1 + w_1 \\ v_2 + w_2 \\ v_3 + w_3 \end{pmatrix} .$$



Vector scaling (multiplication with $a \in \mathbb{R}$): $a \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} = \begin{pmatrix} av_1 \\ av_2 \\ av_3 \end{pmatrix} .$

Dot product, length, angle, orthogonality, unit vectors

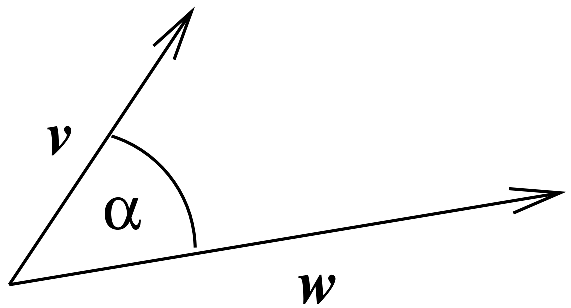
Dot (inner, scalar) product of two vectors: $\boldsymbol{v} \cdot \boldsymbol{w} = \sum_j v_j w_j$.

$$\begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} \cdot \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix} = (v_1, v_2, v_3) \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix} = v_1 w_1 + v_2 w_2 + v_3 w_3 \ .$$

Length of a vector: $\|\boldsymbol{v}\| = \sqrt{\boldsymbol{v} \cdot \boldsymbol{v}}$.
Also: magnitude, (euclidean) norm, $|\boldsymbol{v}|$, v.

Angle between two vectors:

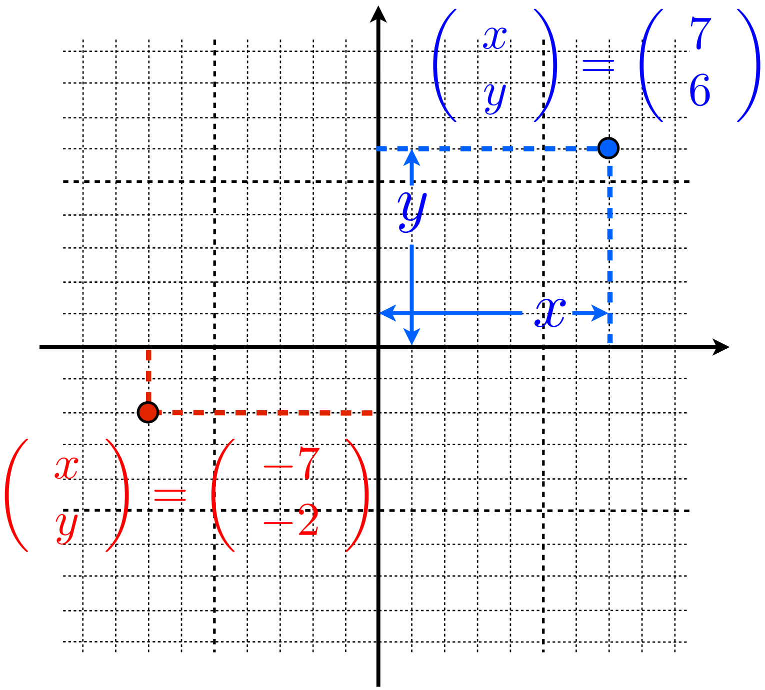
$$\cos\alpha = \cos\angle(\boldsymbol{v}, \boldsymbol{w}) = \frac{\boldsymbol{v} \cdot \boldsymbol{w}}{vw} \ .$$



Perpendicular vectors ($\alpha = 90^\circ$): $\boldsymbol{v} \cdot \boldsymbol{w} = 0$.
Such pairs of vectors are also called *orthogonal*.

Unit vectors ($\hat{\cdot}$) are vectors of unit length (directions): $\hat{\boldsymbol{v}}$, $\hat{\boldsymbol{w}}$, $\hat{\boldsymbol{x}}$, ...

Point coordinates, position vectors, difference vectors



The cartesian *coordinates of a point* denote distances from coordinate lines ($\mathbb{R}^2$) or coordinate planes ($\mathbb{R}^3$):

- x, y (two-dim. space $\mathbb{R}^2$),
- x, y, z (three-dim. space $\mathbb{R}^3$).

Position vector:

$$\boldsymbol{r} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} = x\hat{\boldsymbol{x}} + y\hat{\boldsymbol{y}} + z\hat{\boldsymbol{z}} \; .$$

Difference vector: suppose the

- position vector $\boldsymbol{r}_1$ points from the origin to a point P_1, and the
- position vector $\boldsymbol{r}_2$ points from the origin to a point P_2 , then the
- difference vector $\boldsymbol{r}_2 - \boldsymbol{r}_1$ points from P_1 to P_2.

Difference vectors, lenghts and angles

The distance of a point to the origin is the length of its position vector.

To compute the *distance between two arbitrary points*,

- form position vectors $\boldsymbol{r}_1 = (x_1, y_1, z_1)^\mathsf{T}$ and $\boldsymbol{r}_2 = (x_2, y_2, z_2)^\mathsf{T}$,
- compute the *difference vector* $\boldsymbol{r}_2 - \boldsymbol{r}_1$, and then
- its norm $\|\boldsymbol{r}_2 - \boldsymbol{r}_1\| = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2 + (z_2 - z_1)^2}$.

The angle between two position vectors is the angle at the origin in the corresponding triangle.

To compute an *angle in a triangle formed by three arbitrary points*,

- form the position vector $\boldsymbol{r}_0$ for the point where the angle is located,
- form position vectors $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ for the other two points,
- form the *difference vectors* $\boldsymbol{d}_1 = \boldsymbol{r}_1 - \boldsymbol{r}_0$ and $\boldsymbol{d}_2 = \boldsymbol{r}_2 - \boldsymbol{r}_0$,
- compute the cosine of the angle between $\boldsymbol{d}_1$ and $\boldsymbol{d}_2$ as the dot product $\boldsymbol{d}_1 \cdot \boldsymbol{d}_2$ divided by the lengths $\|\boldsymbol{d}_1\|$ and $\|\boldsymbol{d}_2\|$.

Sample problems

Dot products of vectors, lengths and angles

Compute the angles $\alpha = \angle(\boldsymbol{v}, \boldsymbol{w})$ between the vectors $\boldsymbol{v}$ and $\boldsymbol{w}$.

(a) $\boldsymbol{v} = (2, 0, -2)^\mathsf{T}$, $\boldsymbol{w} = (2, 2, 0)^\mathsf{T}$.
(b) $\boldsymbol{v} = (1, 2, 2)^\mathsf{T}$, $\boldsymbol{w} = (2, 1, -2)^\mathsf{T}$.
(c) $\boldsymbol{v} = (1, 1, -2)^\mathsf{T}$, $\boldsymbol{w} = (-2, -2, 4)^\mathsf{T}$.

Distances and angles in a triangle in $\mathbb{R}^3$

The vertices of a triangle in $\mathbb{R}^3$ are at the position vectors

$$\boldsymbol{r}_1 = \begin{pmatrix} -2 \\ 0 \\ -1 \end{pmatrix}, \quad \boldsymbol{r}_2 = \begin{pmatrix} -2 \\ 0 \\ 3 \end{pmatrix}, \quad \boldsymbol{r}_3 = \begin{pmatrix} -1 \\ \sqrt{2} \\ 2 \end{pmatrix}.$$

Compute the lengths of the three sides and also the angles in the triangle.

Solutions of the sample problems

Dot products of vectors, lengths and angles

The angle between the vectors $\boldsymbol{v}$ and $\boldsymbol{w}$ is given by

$$\alpha \;=\; \angle(\boldsymbol{v},\boldsymbol{w}) \;=\; \arccos\left(\frac{\boldsymbol{v}\cdot\boldsymbol{w}}{vw}\right) \;=\; \arccos\left(\frac{\boldsymbol{v}\cdot\boldsymbol{w}}{|\boldsymbol{v}|\,|\boldsymbol{w}|}\right)$$

hence we have to compute the norms of the vectors as well as the dot product.

For the vectors in (a), $\boldsymbol{v}\cdot\boldsymbol{w} \;=\; 2\cdot 2+0\cdot 2+(-2)\cdot 0 \;=\; 4$, and

$$|\boldsymbol{v}| \;=\; \sqrt{2^2+0^2+(-2)^2} \;=\; \sqrt{8} \;=\; 2\sqrt{2}\ ,$$
$$|\boldsymbol{w}| \;=\; \sqrt{2^2+2^2+0^2} \;=\; \sqrt{8} \;=\; 2\sqrt{2}\ .$$

This gives $\cos\alpha = \dfrac{4}{8} = \dfrac{1}{2}$, and thus $\alpha = \dfrac{\pi}{3} = 60^\circ$.

For the vectors in (b), $\boldsymbol{v}\cdot\boldsymbol{w} \;=\; 1\cdot 2+2\cdot 1+2\cdot(-2) \;=\; 4-4 \;=\; 0$, and $|\boldsymbol{v}| = \sqrt{1^2+2^2+2^2} \;=\; \sqrt{9} \;=\; 3$, $|\boldsymbol{w}| = \sqrt{2^2+1^2+(-2)^2} \;=\; \sqrt{9} \;=\; 3$. This gives $\cos\alpha = 0/9 = 0$, and thus $\alpha = \pi/2 = 90^\circ$.

For the vectors in (c), $\boldsymbol{v}\cdot\boldsymbol{w} \;=\; 1\cdot(-2)+1\cdot(-2)+(-2)\cdot 4 \;=\; -12$, and $|\boldsymbol{v}| = \sqrt{1^2+1^2+(-2)^2} \;=\; \sqrt{6}$, $|\boldsymbol{w}| = \sqrt{(-2)^2+(-2)^2+4^2} \;=\; \sqrt{24} \;=\; 2\sqrt{6}$. This gives $\cos\alpha = -12/12 = -1$, and thus $\alpha = \pi = 180^\circ$.

Solutions of the sample problems

Distances and angles in a triangle in $\mathbb{R}^3$

Define $\boldsymbol{d}_{12} = \boldsymbol{r}_2 - \boldsymbol{r}_1 = \begin{pmatrix} 0 \\ 0 \\ 4 \end{pmatrix}$, $\boldsymbol{d}_{13} = \boldsymbol{r}_3 - \boldsymbol{r}_1 = \begin{pmatrix} 1 \\ \sqrt{2} \\ 3 \end{pmatrix}$, $\boldsymbol{d}_{23} = \boldsymbol{r}_3 - \boldsymbol{r}_2 = \begin{pmatrix} 1 \\ \sqrt{2} \\ -1 \end{pmatrix}$, $\boldsymbol{d}_{31} = \boldsymbol{r}_1 - \boldsymbol{r}_3 = -\boldsymbol{d}_{13}$, $\boldsymbol{d}_{21} = \boldsymbol{r}_1 - \boldsymbol{r}_2 = -\boldsymbol{d}_{12}$, $\boldsymbol{d}_{32} = \boldsymbol{r}_2 - \boldsymbol{r}_3 = -\boldsymbol{d}_{23}$ (difference vectors $\boldsymbol{d}_{jk}$ point from $\boldsymbol{r}_j$ to $\boldsymbol{r}_k$). Side lengths are distances between pairs of points that in turn are the lengths of the difference vectors:

$$|\boldsymbol{d}_{12}| = 4 = |\boldsymbol{d}_{21}| \ , \ |\boldsymbol{d}_{13}| = \sqrt{12} = |\boldsymbol{d}_{31}| \ , \ |\boldsymbol{d}_{23}| = 2 = |\boldsymbol{d}_{32}| \ .$$

Angles (α_j in the corner at position vector $\boldsymbol{r}_j$):

$$\begin{aligned}
\cos\alpha_1 &= \cos\angle(\boldsymbol{d}_{12}, \boldsymbol{d}_{13}) = \frac{\boldsymbol{d}_{12} \cdot \boldsymbol{d}_{13}}{|\boldsymbol{d}_{12}| \cdot |\boldsymbol{d}_{13}|} = \frac{12}{4 \cdot \sqrt{12}} = \frac{3}{2\sqrt{3}} = \frac{\sqrt{3}}{2} \ , \\
\cos\alpha_2 &= \cos\angle(\boldsymbol{d}_{21}, \boldsymbol{d}_{23}) = \frac{1}{2} \ , \\
\cos\alpha_3 &= \cos\angle(\boldsymbol{d}_{31}, \boldsymbol{d}_{32}) = 0 \ ,
\end{aligned}$$

thus $\alpha_1 = \frac{\pi}{3} = 60^\circ$, $\alpha_2 = \frac{\pi}{6} = 30^\circ$. $\alpha_3 = \frac{\pi}{2} = 90^\circ$.

Tangential and orthogonal components of a vector

One often needs to find the *tangential and orthogonal* components of a vector $\boldsymbol{v}$ with respect *to a given direction* $\hat{\boldsymbol{s}}$ (unit vector: $\|\hat{\boldsymbol{s}}\| = 1$).

The tangential component $\boldsymbol{v}_{\|}$ (a vector parallel to $\hat{\boldsymbol{s}}$) is given by

$$\boldsymbol{v}_{\|} \;=\; v_{\|}\,\hat{\boldsymbol{s}} \;=\; (\boldsymbol{v}\cdot\hat{\boldsymbol{s}})\,\hat{\boldsymbol{s}}$$

where $v_{\|} = \boldsymbol{v}\cdot\hat{\boldsymbol{s}}$ is a scalar. The component $\boldsymbol{v}_{\perp}$ orthogonal to $\hat{\boldsymbol{s}}$ is

$$\boldsymbol{v}_{\perp} \;=\; \boldsymbol{v} \;-\; \boldsymbol{v}_{\|}\ .$$

More general, we may be interested to find the components that are *tangential and orthogonal to a linear subspace* $\mathcal{L}$. We suppose that $\{\hat{\boldsymbol{s}}_1, \hat{\boldsymbol{s}}_2, \ldots\}$ is a set of mutually orthogonal unit basis vectors of $\mathcal{L}$.

Tangential component $\boldsymbol{v}_{\|}$ (contained in $\mathcal{L}$): $\boldsymbol{v}_{\|} \;=\; \sum_k (\boldsymbol{v}\cdot\hat{\boldsymbol{s}}_k)\,\hat{\boldsymbol{s}}_k\ .$

Orthogonal component $\boldsymbol{v}_{\perp}$ (perpendicular to $\mathcal{L}$): $\boldsymbol{v}_{\perp} \;=\; \boldsymbol{v} - \boldsymbol{v}_{\|}\ .$

Distances between points and extended geometric objects

The distance of a point P_* to a geometric object (manifold) $\mathcal{M}$ is the smallest possible distance (infimum) between P_* and any point $P \in \mathcal{M}$.

Distance between a point P_* and a curve $\mathcal{C}$: Suppose $\mathcal{C}$ is parametrized by $\boldsymbol{r}(t)$, $t \in \mathbb{R}$, and $\boldsymbol{r}_*$ is the position vector of P_*. Minimizing the square distance $D^2 = \|\boldsymbol{r}(t) - \boldsymbol{r}_*\|^2$ w.r.t. the curve parameter t yields

$$0 \;=\; \frac{\mathrm{d}D^2}{\mathrm{d}t} \;=\; 2\left[\boldsymbol{r}(t) - \boldsymbol{r}_*\right] \cdot \dot{\boldsymbol{r}}(t) \;,$$

hence $\dot{\boldsymbol{r}}(t) \perp \boldsymbol{r}(t) - \boldsymbol{r}_*$ at the position vector $\boldsymbol{r}(t)$ with minimum distance: *The vector pointing from $\boldsymbol{r}(t)$ to $\boldsymbol{r}_*$ is orthogonal to the tangent vector*.[1]

Distance between a point P_* and a two-dimensional surface $\mathcal{S}$:
At the position vector $\boldsymbol{r}(t_1, t_2)$ on $\mathcal{S}$ where the distance is minimum, *the vector pointing from $\boldsymbol{r}(t_1, t_2)$ to $\boldsymbol{r}_*$ is orthogonal to the tangent space*.[2]

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[1] If instead of $t \in \mathbb{R}$ the curve parameter t takes values from a finite interval. i.e., $t \in \mathcal{I} = [a, b]$, the orthogonality condition does not hold at boundary points $\boldsymbol{r}(a), \boldsymbol{r}(b)$.

[2] The tangent space is spanned by the tangent vectors $\partial\boldsymbol{r}/\partial t_1$ and $\partial\boldsymbol{r}/\partial t_2$.

Distance of a point to a linear subspace

The orthogonality condition for the distance between a point P_* and a two-dimensional surface in $\mathbb{R}^3$ translates directly to the general case of the distance between a point P_* and a geometric object (manifold) $\mathcal{M}$ of arbitrary dimension K in N-dim euclidean space $\mathbb{R}^N$.

At the position vector $\boldsymbol{r}_{\text{min}}$ on $\mathcal{M}$ where the distance is minimum,

- *the vector from $\boldsymbol{r}_{min}$ to $\boldsymbol{r}_*$ is orthogonal to the tangent space*.

In the special case of a (K-dimensional) *linear subspace* $\mathcal{L}$ of $\mathbb{R}^N$ (e.g., line or plane through the origin) with an orthonormal basis $\{\hat{\boldsymbol{s}}_1, \hat{\boldsymbol{s}}_2, \ldots, \hat{\boldsymbol{s}}_K\}$ (set of K mutually orthogonal unit basis vectors) of $\mathcal{L}$, we find that

- the tangential component of $\boldsymbol{r}_*$ is the vector $\boldsymbol{r}_{\text{min}}$ on $\mathcal{L}$ where the distance is minimum, i.e., $\boldsymbol{r}_{\text{min}} = \boldsymbol{r}_{*,\parallel} = \sum_k (\boldsymbol{r}_* \cdot \hat{\boldsymbol{s}}_k)\hat{\boldsymbol{s}}_k$,
- the orthogonal component of $\boldsymbol{r}_*$ is the distance vector $\boldsymbol{r}_* - \boldsymbol{r}_{\text{min}}$ (pointing from $\boldsymbol{r}_{\text{min}}$ to $\boldsymbol{r}_*$): $\boldsymbol{r}_* - \boldsymbol{r}_{\text{min}} = \boldsymbol{r}_{*,\perp} = \boldsymbol{r}_* - \sum_k (\boldsymbol{r}_* \cdot \hat{\boldsymbol{s}}_k)\hat{\boldsymbol{s}}_k$,
- the distance $D(P_*, \mathcal{L})$ is the length $\|\boldsymbol{r}_* - \boldsymbol{r}_{\text{min}}\|$ of the distance vector.

Sample problems

Distance of a point to linear subspaces

Determine the distance of the point P_* at $\boldsymbol{r}_* = (5, -12, 10)^\mathsf{T}$ to the

(a) line parametrized by $\boldsymbol{r}(t) = t(4, 0, 3)^\mathsf{T}$,
(b) plane described by the equation $x - 2y - 2z = 0$,
(c) plane parametrized by $\boldsymbol{r}(t_1, t_2) = t_1(4, 0, 3)^\mathsf{T} + t_2(0, 5, 0)^\mathsf{T}$.

Distance of a point to a parabola

The position vector $\boldsymbol{r}_*$ of a point P_* on the y-axis and the curve $\mathcal{C}$ are given by $\boldsymbol{r}_* = \begin{pmatrix} 0 \\ y_* \end{pmatrix}$ and $\boldsymbol{r}(t) = \begin{pmatrix} x(t) \\ y(t) \end{pmatrix} = \begin{pmatrix} t \\ t^2 \end{pmatrix}$ for $t \in \mathbb{R}$, respectively.

(a) Determine the distance $D(P_*, \mathcal{C})$ as a function of t. Set the derivative to zero to find the coordinates of P_{min} on $\mathcal{C}$ with minimum distance.
(b) Verify the orthogonality of tangent vector and distance vector at P_{min}.

Solutions of the sample problems

Distance of a point to linear subspaces

Position vector of point P_*: $\boldsymbol{r}_* = (5, -12, 10)^\mathsf{T}$.

(a) Line $\boldsymbol{r}(t) = t\boldsymbol{v}$, tangent vector $\boldsymbol{v} = (4, 0, 3)^\mathsf{T}$. Unit tangent vector: $\hat{\boldsymbol{v}} = \boldsymbol{v}/5$.

- Tangential component of $\boldsymbol{r}_*$: $\boldsymbol{r}_{*,\parallel} = (\boldsymbol{r}_* \cdot \hat{\boldsymbol{v}})\hat{\boldsymbol{v}} = 10\hat{\boldsymbol{v}} = (8, 0, 6)^\mathsf{T}$.
- Orthogonal component: $\boldsymbol{r}_{*,\perp} = \boldsymbol{r}_* - \boldsymbol{r}_{*,\parallel} = (-3, -12, 4)^\mathsf{T}$.
- Distance: $\|\boldsymbol{r}_{*,\perp}\| = \sqrt{9 + 144 + 16} = 13$.

(b) Plane described by the equation $x - 2y - 2v = 0$.

- Normal vector $\boldsymbol{n} = (1, -2, -2)^\mathsf{T}$ (orthogonal to plane).
- Unit normal vector: $\hat{\boldsymbol{n}} = \boldsymbol{n}/3$.
- Orthogonal component of $\boldsymbol{r}_*$: $\boldsymbol{r}_{*,\perp} = (\boldsymbol{r}_* \cdot \hat{\boldsymbol{n}})\hat{\boldsymbol{n}} = 3\hat{\boldsymbol{n}} = (1, -2, -2)^\mathsf{T}$.
- Distance: $\|\boldsymbol{r}_{*,\perp}\| = |\boldsymbol{r}_* \cdot \hat{\boldsymbol{n}}| = 3$.

(c) Plane $\boldsymbol{r}(t_1, t_2) = t_1\boldsymbol{v}_1 + t_2\boldsymbol{v}_2$, tangent vectors $\boldsymbol{v}_1 = (4, 0, 3)^\mathsf{T}, \boldsymbol{v}_2 = (0, 5, 0)^\mathsf{T}$.

- Unit normal vector $\hat{\boldsymbol{n}} = \hat{\boldsymbol{v}}_1 \times \hat{\boldsymbol{v}}_2 = \frac{1}{5}(-3, 0, 4)^\mathsf{T}$.
- Orthogonal component of $\boldsymbol{r}_*$: $\boldsymbol{r}_{*,\perp} = (\boldsymbol{r}_* \cdot \hat{\boldsymbol{n}})\hat{\boldsymbol{n}} = 5\hat{\boldsymbol{n}} = (-3, 0, 4)^\mathsf{T}$.
- Distance: $\|\boldsymbol{r}_{*,\perp}\| = |\boldsymbol{r}_* \cdot \hat{\boldsymbol{n}}| = 5$.

Solutions of the sample problems

Distance of a point to a parabola

Position vector: $\boldsymbol{r}_* = \begin{pmatrix} 0 \\ y_* \end{pmatrix}$. Curve $\mathcal{C}$: $\boldsymbol{r}(t) = \begin{pmatrix} x(t) \\ y(t) \end{pmatrix} = \begin{pmatrix} t \\ t^2 \end{pmatrix}$.

(a) Distance $D(P_*, \mathcal{C})$ as a function of t: $D_*(t) = \sqrt{t^2 + (t^2 - y_*)^2}$. The derivative $D'_*(t) = t[1 + 2(t^2 - y_*)]/D_*(t) = 2t[t^2 - (y_* - \frac{1}{2})]/D_*(t)$ is zero if $0 = t[t^2 - (y_* - \frac{1}{2})] = t\left(t + \sqrt{y_* - \frac{1}{2}}\right)\left(t - \sqrt{y_* - \frac{1}{2}}\right)$, i.e., if $t = t_0 = 0$ or $t = t_{1,2} = \pm\sqrt{y_* - \frac{1}{2}}$. If $y_* \leq \frac{1}{2}$, then $t = t_0$ and the minimum distance is assumed at $\boldsymbol{r}_{\text{min}} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$, otherwise $t = t_{1,2}$ and $\boldsymbol{r}_{\text{min}} = \begin{pmatrix} \pm\sqrt{y_* - \frac{1}{2}} \\ y_* - \frac{1}{2} \end{pmatrix}$.

(b) Tangent vector: $\dot{\boldsymbol{r}}(t) = \begin{pmatrix} 1 \\ 2t \end{pmatrix}$. Distance vector for the case

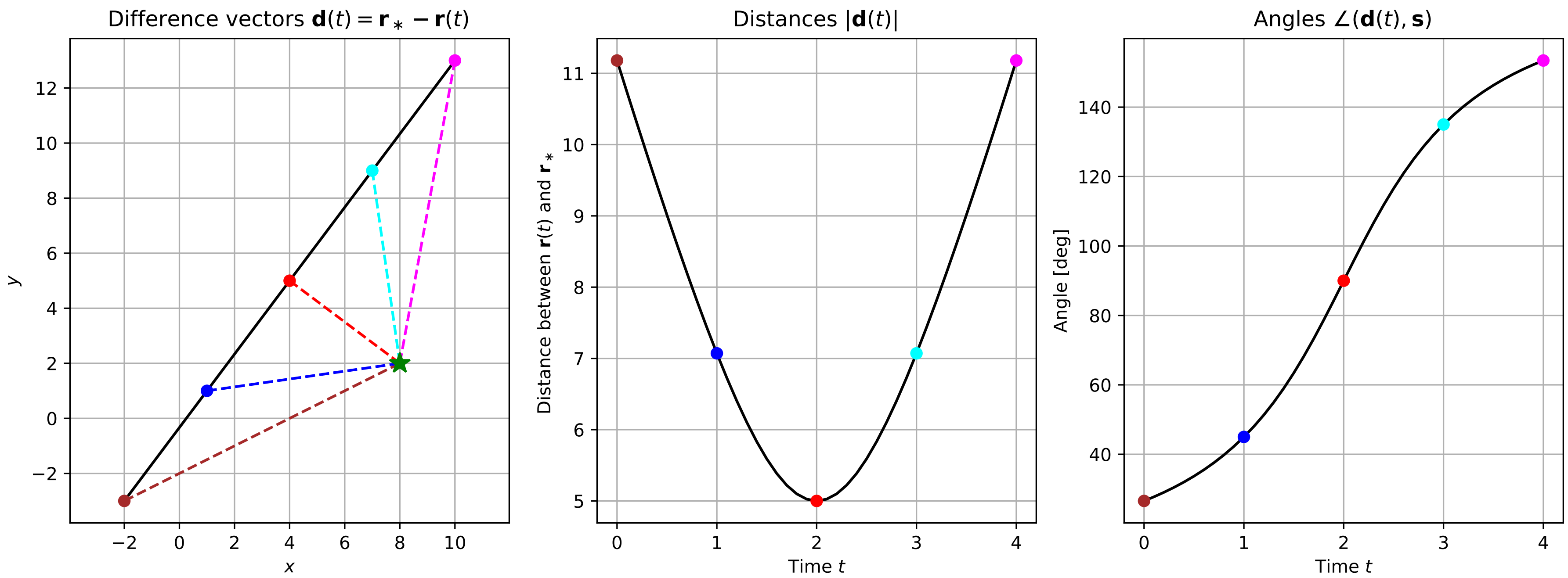
- $y_* \leq \frac{1}{2}$: $\boldsymbol{r}_* - \boldsymbol{r}_{\text{min}} = \begin{pmatrix} 0 \\ y_* \end{pmatrix} \perp \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \dot{\boldsymbol{r}}(t = 0)$.
- $y_* > \frac{1}{2}$: $\boldsymbol{r}_* - \boldsymbol{r}_{\text{min}} = \begin{pmatrix} \mp\sqrt{y_* - 1} \\ \frac{1}{2} \end{pmatrix} \perp \begin{pmatrix} 1 \\ \pm 2\sqrt{y_* - 1} \end{pmatrix} = \dot{\boldsymbol{r}}(t = t_{1,2})$.

Vector operations, difference vectors, distances, angles

- Python/NumPy implementation of vectors and vector operations
- Difference vectors and distances, dot products and angles

Minimum distances between points and geometric objects

- Tangential and orthogonal components of a vector w.r.t. linear subspaces
- Illustration of the orthogonality principle



Vector algebra concepts in data analysis and modeling

Data vectors, mean and variance

Data sets can be understood as data vectors

Samples of N measurements $\{u_1, u_2, \ldots, u_N\}$ and $\{v_1, v_2, \ldots, v_N\}$ can be interpreted as *data vectors* in N-dimensional (euclidean) space:

$$\boldsymbol{u} = \begin{pmatrix} u_1 \\ \vdots \\ u_N \end{pmatrix}, \ \boldsymbol{v} = \begin{pmatrix} v_1 \\ \vdots \\ v_N \end{pmatrix}.$$

Mean and variance

The *mean* $\bar{u} = \frac{1}{N}\sum_k u_k$ and the *variance* $(\Delta u)^2 = \frac{1}{N}\sum_k (u_k - \bar{u})^2$ of a data set can be geometrically characterized as follows.

- The tangential component $\boldsymbol{u}_\parallel = (\boldsymbol{u} \cdot \hat{\boldsymbol{e}})\hat{\boldsymbol{e}}$ of the data vector $\boldsymbol{u}$ in the direction of $\boldsymbol{e} = (1, 1, \ldots, 1)^\mathsf{T}$ (unit vector $\hat{\boldsymbol{e}} = \boldsymbol{e}/\sqrt{N}$) is the constant data vector $(\bar{u}, \bar{u}, \ldots, \bar{u})^\mathsf{T}$.
- Subtracting the mean gives the orthogonal component $\boldsymbol{u}_\perp = \boldsymbol{u} - \boldsymbol{u}_\parallel$.
- Variance: $(\Delta u)^2 = \frac{1}{N}\|\boldsymbol{u}_\perp\|^2$.

Covariance and correlation

Covariance of two data sets u and v: $\text{cov}(u, v) = \frac{1}{N} \sum_k (u_k - \bar{u})(v_k - \bar{v})$.

The covariance is $\frac{1}{N}$ times the scalar product of the data vector components $\boldsymbol{u}_\perp$ and $\boldsymbol{v}_\perp$ orthogonal to $\boldsymbol{e} = (1, 1, \ldots, 1)^\mathsf{T}$:

$$\text{cov}(u, v) \;=\; \frac{1}{N}\, \boldsymbol{u}_\perp \cdot \boldsymbol{v}_\perp \;.$$

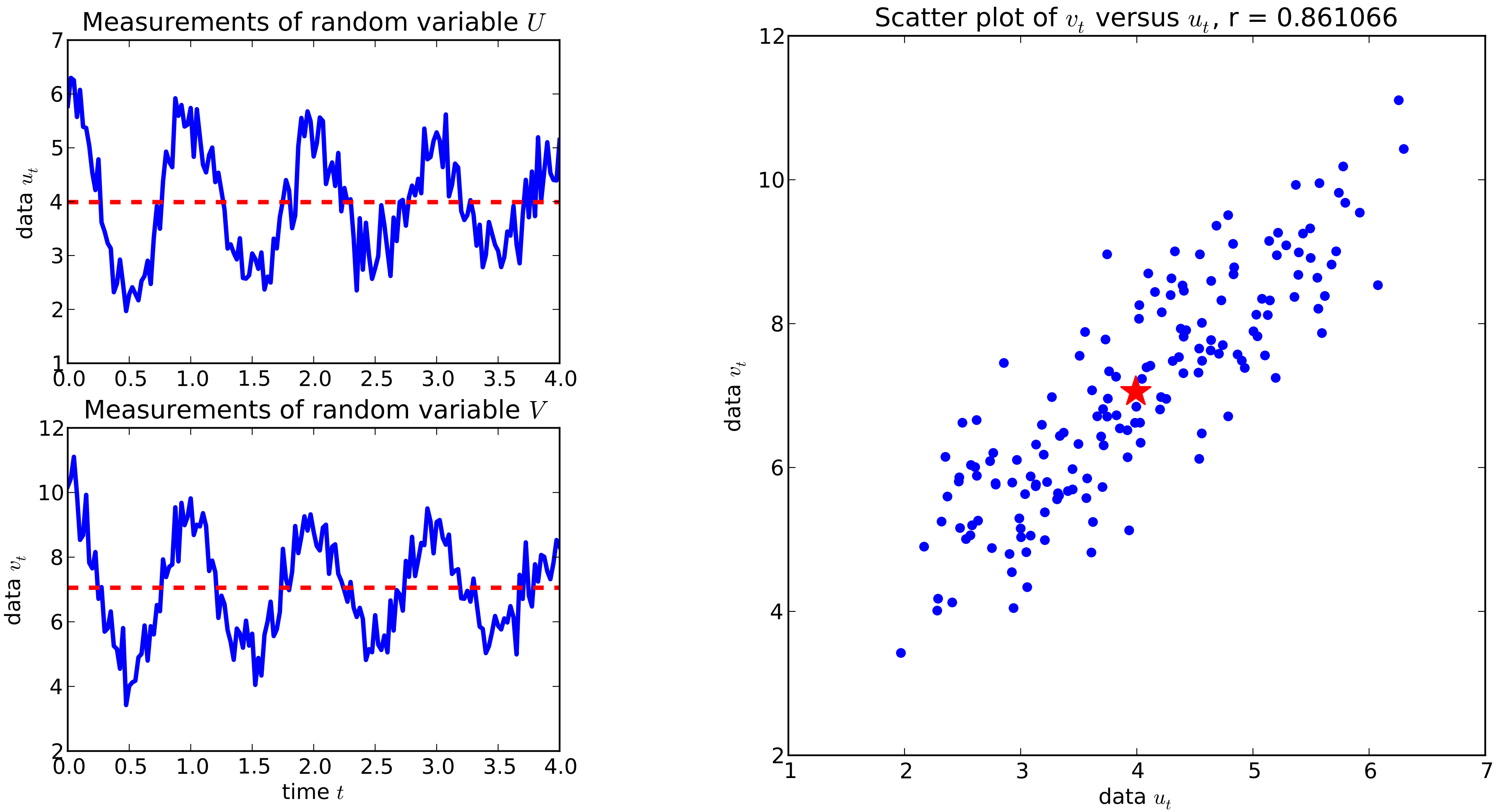
Pearson's correlation coefficient $r = r(u, v)$:

$$r(u, v) \;=\; \frac{\text{cov}(u, v)}{\Delta u \cdot \Delta v} \;=\; \frac{\boldsymbol{u}_\perp \cdot \boldsymbol{v}_\perp}{\|\boldsymbol{u}_\perp\| \cdot \|\boldsymbol{v}_\perp\|} \;=\; \cos \angle\left(\boldsymbol{u}_\perp, \boldsymbol{v}_\perp\right) \;.$$

The coefficient $r \in [-1, 1]$ is a measure of *linear correlation*.

Values close $\left\{ \begin{array}{c} 1 \\ 0 \\ -1 \end{array} \right\}$ suggest that the variables are $\left\{ \begin{array}{c} \text{correlated} \\ \text{uncorrelated} \\ \text{anti-correlated} \end{array} \right\}$.

Illustration of correlated time series



Data space and model space

Data modeling: assume the observed *data* d result from a deterministic *model* m and a *random component* r (residual). Independent variable t: d_t, $d(t)$, m_t, ...

- Model equations: $d_t = m_t + r_t$ or $d(t) = m(t) + r(t)$.
- To make model parameters (vector $\boldsymbol{\omega}$) explicit, write $m = m(t|\boldsymbol{\omega})$.
- Interpret d_t, m_t, r_t as components of vectors $\boldsymbol{d}$, $\boldsymbol{m}$, $\boldsymbol{r}$, then $\boldsymbol{d} = \boldsymbol{m} + \boldsymbol{r}$.

Data space $\mathcal{D}$ and model space $\mathcal{M}$

Important numbers: N is the total number of measurements, and K is the number of independent model parameters (components of vector $\boldsymbol{\omega}$).

- The data vector $\boldsymbol{d}$ lives in a linear space of dimension N, the *data space* $\mathcal{D}$.
- The model vector $\boldsymbol{m}$ can access only a part of $\mathcal{D}$ as specified by m and $\boldsymbol{\omega}$. This part of $\mathcal{D}$ is the *model space* $\mathcal{M}$, a K-dimensional submanifold of $\mathcal{D}$.

If all parameters $a_1, a_2, \ldots$ enter the model function $m = m(t|\boldsymbol{a})$ linearly, they are called amplitudes, and $\mathcal{M}$ forms a *linear subspace* of $\mathcal{D}$. The model function can then be written in the form $m(t|\boldsymbol{a}) = \sum_{k=1}^{K} a_k f_k(t)$. The functions $f_k = f_k(t)$, $k = 1, 2, 3, \ldots$, are called *basis functions*.

Geometrical characterization of the least squares principle

Least squares approach to data modeling: the optimum model is found by minimizing the error-weighted square deviation of data and model.

$$\chi^2 = \sum_t \left(\frac{d(t) - m(t|\boldsymbol{\omega})}{\sigma_t} \right)^2 = \sum_t \left(\frac{r(t|\boldsymbol{\omega})}{\sigma_t} \right)^2 \stackrel{!}{=} \text{Min} .$$

Assuming constant measurement errors, $\sigma_t = \sigma_0 = \text{const}$, we obtain

$$\chi^2 \propto \|\boldsymbol{r}\|^2 = \|\boldsymbol{d} - \boldsymbol{m}\|^2 \stackrel{!}{=} \text{Min} .$$

Among all admissible model vectors $\boldsymbol{m} \in \mathcal{M}$, the *optimum model* $\boldsymbol{m}_{opt}$

- minimizes the (square) distance to the data vector $\boldsymbol{d}$, and
- satisfies the *orthogonality condition*: the residual vector $\boldsymbol{r} = \boldsymbol{d} - \boldsymbol{m} = \boldsymbol{d} - \boldsymbol{m}_{\text{opt}}$ is orthogonal to the tangent space of $\mathcal{M}$.

Linear models $m = m(t|\boldsymbol{a})$: $\mathcal{M}$ is a linear subspace of $\mathcal{D}$.

- Optimum model $\boldsymbol{m}_{\text{opt}} = \boldsymbol{d}_{\|}$: component of $\boldsymbol{d}$ tangential to $\mathcal{M}$.
- Residual $\boldsymbol{r} = \boldsymbol{d}_{\perp}$: component of $\boldsymbol{d}$ orthogonal $\mathcal{M}$.

Least squares solution for linear models

The amplitudes $a_1, a_2, \ldots, a_K$ of the linear model $m(t|\boldsymbol{a}) = \sum_{k=1}^{K} a_k f_k(t)$ that are optimum in the least squares sense can be found from N $(> K)$ measurements at $t_1, t_2, \ldots, t_N$ through the solution of $\mathbf{M}\boldsymbol{a} = \boldsymbol{d}$ where

- $\mathbf{M}$ is the $N \times K$ *design matrix* with elements $M_{nk} = f_k(t_n)$,
- $\boldsymbol{a} = (a_1, a_2, \ldots, a_K)^\mathsf{T}$ is the vector of *K model parameters*,
- $\boldsymbol{d} = (d_1, d_2, \ldots, d_N)^\mathsf{T}$ comprises *N measured values*.

The amplitude vector $\boldsymbol{a}$ is given by the so-called normal equation

$$\boldsymbol{a} \;=\; \left(\mathbf{M}^\mathsf{T}\mathbf{M}\right)^{-1} \mathbf{M}^\mathsf{T}\boldsymbol{d} \;=\; \mathbf{M}^{\mathsf{ils}}\boldsymbol{d} \quad \text{with} \quad \mathbf{M}^{\mathsf{ils}} \;=\; \left(\mathbf{M}^\mathsf{T}\mathbf{M}\right)^{-1} \mathbf{M}^\mathsf{T}\,.$$

The matrix $\mathbf{M}^{\mathsf{ils}}$ is the pseudo-inverse of $\mathbf{M}$ in the least-squares sense.

Orthogonal basis functions: If the K column vectors of the design matrix $\boldsymbol{f}_k = (f_k(t_1), f_k(t_2), \ldots, f_k(t_N))^\mathsf{T}$ yield an orthogonal ($\boldsymbol{f}_k \cdot \boldsymbol{f}_\ell = 0$ if $k \neq \ell$) basis of the model space $\mathcal{M}$, the amplitude estimates are

$$a_k \;=\; \frac{\boldsymbol{d} \cdot \boldsymbol{f}_k}{\|\boldsymbol{f}_k\|^2} \;=\; \frac{\boldsymbol{d} \cdot \boldsymbol{f}_k}{\boldsymbol{f}_k \cdot \boldsymbol{f}_k}\,.$$

Sample problems

Least squares estimate of an invariant parameter

Suppose at times $t_1, t_2, \ldots, t_N$ the measurements $d_1, d_2, \ldots, d_N$ of an invariant parameter μ are taken in the presence of noise r_t: $d_t = m_t + r_t$. The model function is thus simply $m(t|\mu) = \mu$. The measurement errors σ do not change with t. Compute the least squares estimate of μ.

Parameters of a regression line

Suppose N noisy measurements $d_1, d_2, \ldots, d_N$ are taken at times $t_1, t_2, \ldots, t_N$. We wish to obtain least squares estimates of the regression line parameters a_1, a_2 in $m(t|a_1, a_2) = a_1 + a_2(t - t_*)$. The basis functions are $f_1 = 1$ and $f_2 = t - t_*$, and t_* can be adjusted to the problem.

- Determine t_* such that the two basis functions are orthogonal.
- Find least squares estimates of the regression line parameters a_1, a_2.

Solutions of the sample problems

Least squares estimate of an invariant parameter

Since $m(t|\mu) = \mu = \mu f(t)$ with the (basis) function $f(t) = 1$, $\boldsymbol{f} \cdot \boldsymbol{f} = N$ and $\boldsymbol{d} \cdot \boldsymbol{f} = \sum_n d_n$, we obtain $\mu = \frac{1}{N} \sum_n d_n = \bar{d}$.

Parameters of a regression line

Choosing $t_* = 0$ would usually result in a non-orthogonal set of basis functions. Here we determine t_* through the condition

$$0 = \boldsymbol{f}_1 \cdot \boldsymbol{f}_2 = \sum_n (t_n - t_*) = \sum_n t_n - N t_* \ ,$$

thus $t_* = \frac{1}{N} \sum_n t_n = \bar{t}$ (mean value of measurement times).

Square norms of basis functions: $\|\boldsymbol{f}_1\|^2 = N$ and $\|\boldsymbol{f}_2\|^2 = \sum_n (t_n - \bar{t})^2$, thus $\|\boldsymbol{f}_2\|^2 = N(\Delta t)^2$ where $(\Delta t)^2$ is the variance of measurement times.

Parameters of the regression line $m(t|a_1, a_2) = a_1 + a_2(t - \bar{t})$:

$$a_1 = \frac{\boldsymbol{d} \cdot \boldsymbol{f}_1}{\|\boldsymbol{f}_1\|^2} = \frac{1}{N} \sum_n d_n = \bar{d} \ , \ a_2 = \frac{\boldsymbol{d} \cdot \boldsymbol{f}_2}{\|\boldsymbol{f}_2\|^2} = \frac{\sum_n d_n (t_n - \bar{t})}{\sum_n (t_n - \bar{t})^2} \ .$$

Orthogonality condition and least squares solution

Orthogonality condition in statistical data modeling

Suppose $\boldsymbol{m}' = \boldsymbol{m}_{\text{opt}} + \delta\boldsymbol{m}$ is an admissible alternative ($\boldsymbol{m}' \in \mathcal{M}$) of the optimum model $\boldsymbol{m}_{\text{opt}}$ obtained through a perturbation $\delta\boldsymbol{m}$ (in tangent space: $\boldsymbol{r}_{\text{opt}} \cdot \delta\boldsymbol{m} = 0$). The norm of the resulting residual $\boldsymbol{r}' = \boldsymbol{d} - \boldsymbol{m}' = \boldsymbol{r}_{\text{opt}} - \delta\boldsymbol{m}$ must be larger than $\|\boldsymbol{r}_{\text{opt}}\|$ because

$$\begin{aligned} \|\boldsymbol{r}'\|^2 &= (\boldsymbol{r}_{\text{opt}} - \delta\boldsymbol{m}) \cdot (\boldsymbol{r}_{\text{opt}} - \delta\boldsymbol{m}) \;=\; \|\boldsymbol{r}_{\text{opt}}\|^2 \;-\; 2\boldsymbol{r}_{\text{opt}} \cdot \delta\boldsymbol{m} \;+\; \|\delta\boldsymbol{m}\|^2 \\ &= \|\boldsymbol{r}_{\text{opt}}\|^2 \;+\; \|\delta\boldsymbol{m}\|^2 \;>\; \|\boldsymbol{r}_{\text{opt}}\|^2 \;. \end{aligned}$$

Parameters of a linear model with respect to an orthonormal basis

Consider the linear model vector $\boldsymbol{m} = \sum_k a_k \hat{\boldsymbol{m}}_k$ where $\hat{\boldsymbol{m}}_1, \hat{\boldsymbol{m}}_2, \ldots$ form an orthonormal basis of $\mathcal{M}$. Then $\boldsymbol{m} \cdot \hat{\boldsymbol{m}}_k = \sum_\ell a_\ell \hat{\boldsymbol{m}}_\ell \cdot \hat{\boldsymbol{m}}_k = a_k$. Furthermore, $\boldsymbol{m} \cdot \hat{\boldsymbol{m}}_k = (\boldsymbol{d} - \boldsymbol{r}) \cdot \hat{\boldsymbol{m}}_k = \boldsymbol{d} \cdot \hat{\boldsymbol{m}}_k$ because $\boldsymbol{r} \perp \hat{\boldsymbol{m}}_k \in \mathcal{M}$, thus $a_k = \boldsymbol{d} \cdot \hat{\boldsymbol{m}}_k$.

The algebra rests on a few key properties, namely, it is required that the dot (scalar) product is (1) symmetric, (2) bilinear, and (3) positive definite:

1. $\boldsymbol{u} \cdot \boldsymbol{v} = \boldsymbol{v} \cdot \boldsymbol{u}$,
2. $(a_1\boldsymbol{u}_1 + a_2\boldsymbol{u}_2) \cdot \boldsymbol{v} = a_1\boldsymbol{u}_1 \cdot \boldsymbol{v} + a_2\boldsymbol{u}_2 \cdot \boldsymbol{v}$,
3. $\boldsymbol{u} \cdot \boldsymbol{u} \geq 0$, and $\boldsymbol{u} \cdot \boldsymbol{u} = 0$ implies $\boldsymbol{u} = \boldsymbol{0}$ (only $\boldsymbol{0}$ has zero norm).

Properties of inner (scalar) products

Linear spaces are collections of objects that can be added and scaled in a meaningful way. Such objects are called *vectors*. Examples: tuples of real or complex numbers, data sets, real-valued or complex-valued functions.

An *inner product* $\langle\cdot|\cdot\rangle$ on a vector space $\mathcal{V}$ over $\mathbb{R}$ is a function $\mathcal{V}\times\mathcal{V}\to\mathbb{R}$ that is (1) symmetric, (2) bilinear, and (3) positive definite. Explicitly, for all $\boldsymbol{u},\boldsymbol{v},\boldsymbol{u}_1,\boldsymbol{u}_2\in\mathcal{V}$ and all $a_1,a_2\in\mathbb{R}$ we require that

1. $\langle\boldsymbol{u}|\boldsymbol{v}\rangle=\langle\boldsymbol{v}|\boldsymbol{u}\rangle$,
2. $\langle a_1\boldsymbol{u}_1+a_2\boldsymbol{u}_2|\boldsymbol{v}\rangle=a_1\langle\boldsymbol{u}_1|\boldsymbol{v}\rangle+a_2\langle\boldsymbol{u}_2|\boldsymbol{v}\rangle$,
3. $\langle\boldsymbol{u}|\boldsymbol{u}\rangle\geq 0$, and $\langle\boldsymbol{u}|\boldsymbol{u}\rangle=0$ implies $\boldsymbol{u}=\mathbf{0}$ (only $\mathbf{0}$ has zero norm).

An inner product allows to define distances and angles between vectors.

- *Norm* (length, magnitude): $\|\boldsymbol{u}\|=\sqrt{\langle\boldsymbol{u}|\boldsymbol{u}\rangle}$.
- *Distance*: $\mathrm{dist}(\boldsymbol{u},\boldsymbol{v})=\|\boldsymbol{u}-\boldsymbol{v}\|$.
- *Angle*: $\cos\angle(\boldsymbol{u},\boldsymbol{v})=\frac{\langle\boldsymbol{u}|\boldsymbol{v}\rangle}{\|\boldsymbol{u}\|\cdot\|\boldsymbol{v}\|}$.

Inner products for vector spaces over $\mathbb{C}$: $\langle\boldsymbol{u}|\boldsymbol{v}\rangle=\langle\boldsymbol{v}|\boldsymbol{u}\rangle^*$ (complex conjugation).

Inner product examples

N-tuples of real numbers (euclidean space $\mathbb{R}^N$): $\langle \boldsymbol{u}|\boldsymbol{v}\rangle = \sum_n u_n v_n$.

N-tuples of complex numbers (euclidean space $\mathbb{C}^N$): $\langle \boldsymbol{u}|\boldsymbol{v}\rangle = \sum_n u_n v_n^*$.

Data sets (real-valued), no error weights: $\langle u|v\rangle = \dfrac{1}{N}\displaystyle\sum_n u_n v_n$.

- $\langle e|e\rangle = 1$ for $e = \{1, 1, \ldots, 1\}$, thus $e = \hat{e}$ (unit vector).
- Mean: $\langle u|e\rangle = \bar{u}$ and $u_\parallel = \langle u|e\rangle\, e = \{\bar{u}, \bar{u}, \ldots, \bar{u}\}$.
- Variance: $\|u_\perp\|^2$ where $u_\perp = u - u_\parallel$.
- Linear correlation coefficient: $r(u, v) = \cos\angle(u_\perp, v_\perp)$.

Data sets (real-valued), error weights σ_n: $\langle u|v\rangle = \dfrac{\sum_n \sigma_n^{-2} u_n v_n}{\sum_n \sigma_n^{-2}}$.

Real-valued functions, weight function w: $\langle f|g\rangle = \int_a^b f(x)\, g(x)\, w(x)\, \mathrm{d}x$.

Complex-valued functions: $\langle f|g\rangle = \int_a^b f(x)\, g^*(x)\, w(x)\, \mathrm{d}x$.

Periodic functions, cosine and sine series

Functions $f = f(t)$ that are *periodic on an interval of length T* (period) can be approximated by *cosine and sine functions*:

$$f(t) \;=\; \frac{C_0}{2} + \sum_k \left\{ C_k \cos\left(\frac{2\pi k t}{T}\right) + S_k \sin\left(\frac{2\pi k t}{T}\right) \right\} + r(t) \;.$$

Define $\omega = 2\pi/T$, $u_k(t) = \cos k\omega t$ and $v_k(t) = \sin k\omega t$ for $k = 1, 2, 3, \ldots$, and $u_0(t) = 1/2$. Then $\{u_0, u_1, v_1, u_2, v_2, \ldots\}$ forms an *orthogonal set of functions* with respect to the inner product

$$\langle f|g\rangle \;=\; \int_0^T f(t)\, g(t)\, \mathrm{d}t \;.$$

Square norms: $\langle u_k|u_k\rangle = \langle v_k|v_k\rangle = T/2$.

Expansion coefficients $C_k = \frac{\langle f|u_k\rangle}{\langle u_k|u_k\rangle}$ and $S_k = \frac{\langle f|v_k\rangle}{\langle v_k|v_k\rangle}$:

$$C_k \;=\; \frac{2}{T}\int_0^T f(t)\,\cos\left(\frac{2\pi k t}{T}\right)\,\mathrm{d}t \;\;,\;\; S_k \;=\; \frac{2}{T}\int_0^T f(t)\,\sin\left(\frac{2\pi k t}{T}\right)\,\mathrm{d}t \;\;.$$

Legendre polynomials

Legendre polynomials $P_n(x)$ are important for the spherical harmonics expansion of geophysical potential fields (gravity, geomagnetism).

The functions $P_n(x), n = 0, 1, 2, \ldots$, are polynomials of degree n with n zeroes in $]-1, 1[$. They form a sequence of *orthogonal functions* on $[-1, 1]$ with respect to the inner product

$$\langle f|g\rangle \;=\; \int_{-1}^{1} f(x)\, g(x)\, \mathrm{d}x \;.$$

The first two Legendre polynomials are $P_0(x) = 1$ and $P_1(x) = x$, and for higher degrees $P_n(x)$ can be obtained from the *recursion formula*

$$(n+1)P_{n+1}(x) \;=\; (2n+1)xP_n(x) - nP_{n-1}(x) \;.$$

Normalization: $\langle P_n|P_n\rangle = \displaystyle\int_{-1}^{1} [P_n(x)]^2 \mathrm{d}x = \frac{2}{2n+1}$.

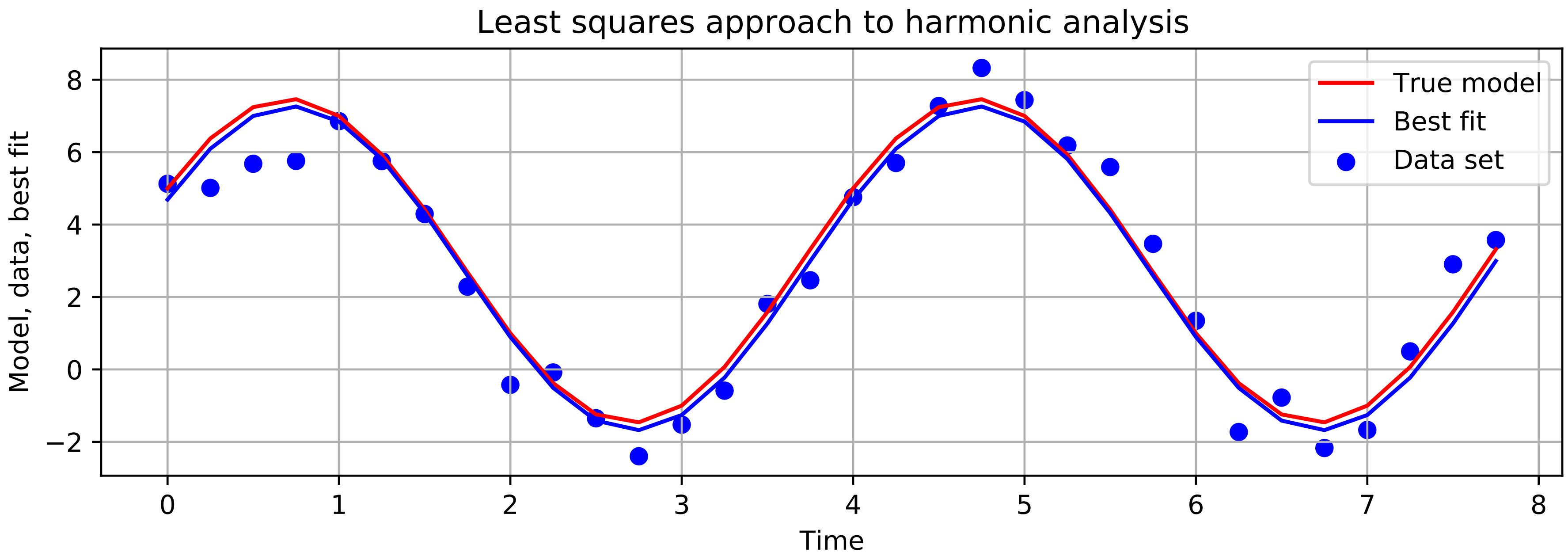
Approximation of functions on $[-1, 1]$: $f(x) \;=\; \sum_n f_n P_n(x) \;+\; r(x)$.

Mean, variance, covariance, correlation

- Illustration of the vector perspective on basic statistics

Geometrical characterization of the least squares principle

- Comparison of orthogonal least squares with `numpy.ployfit()`
- Exercise: least squares fitting of harmonic functions



Linear equations, inversion, matrix decompositions

Matrix transposition and matrix addition

What is a matrix?

- A $n \times m$ *matrix* $\mathbf{A}$ over $\mathbb{R}$ is a rectangular array of real numbers A_{jk} with n rows and m columns.
- Turning the rows of $\mathbf{A}$ into columns and vice-versa results in the *transpose* matrix $\mathbf{A}^\mathsf{T}$. This is a $m \times n$ matrix with entries A_{kj}.
- A vector in $\mathbb{R}^n$ is a $n \times 1$ matrix (column vector $\boldsymbol{a}$).
- A row vector in $\mathbb{R}^n$ is a $1 \times n$ matrix ($\boldsymbol{a}^\mathsf{T}$).

Matrix transposition example

$$\mathbf{A} = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{pmatrix} \quad \Rightarrow \quad \mathbf{A}^\mathsf{T} = \begin{pmatrix} 1 & 4 \\ 2 & 5 \\ 3 & 6 \end{pmatrix} .$$

Matrices are added or multiplied with a scalar value in the same way as vectors (through elementwise operations).

Matrix multiplication

Product of two matrices: Two matrices can be multiplied if the number of columns of the first matrix matches the number of rows of the second matrix. The matrix product $\mathbf{C} = \mathbf{BA}$ is a $n \times p$ matrix if $\mathbf{B}$ is a $n \times m$ matrix and $\mathbf{A}$ is a $m \times p$ matrix. The entries of $\mathbf{C}$ are

$$C_{j\ell} = \sum_{k=1}^{m} B_{jk} A_{k\ell} \; .$$

Matrix multiplication example

$$\begin{pmatrix} 1 & 3 & 5 \\ 2 & 4 & 6 \end{pmatrix} \begin{pmatrix} 1 & 2 & 3 & 4 \\ -2 & -3 & -4 & -5 \\ 3 & 4 & 5 & 6 \end{pmatrix} = \begin{pmatrix} 10 & 13 & 16 & 19 \\ 12 & 16 & 20 & 24 \end{pmatrix}$$

For two vectors $\boldsymbol{a}, \boldsymbol{b} \in \mathbb{R}^n$, the matrix product $\boldsymbol{a}^\mathsf{T}\boldsymbol{b}$ gives the dot (or inner) product of the two vectors[3]: $\boldsymbol{a}^\mathsf{T}\boldsymbol{b} = \sum_{j=1}^{n} a_j b_j = \boldsymbol{a} \cdot \boldsymbol{b}$.

[3] The so-called dyadic (or outer) product $\boldsymbol{a}\boldsymbol{b}^\mathsf{T}$ is a $n \times n$ matrix with elements $a_j b_k$.

Matrix representation of linear equations

Systems of linear equations are conveniently expressed using matrices.

- Unknown variables are assembled in a (column) vector $\boldsymbol{u}$.
- Known values form a (column) vector $\boldsymbol{k}$.
- Coefficients in the equations are the elements of a matrix $\mathbf{C}$.
- *Equivalent matrix equation:* $\mathbf{C}\boldsymbol{u} = \boldsymbol{k}$.
- *Augmented matrix* of the linear system: $(\mathbf{C}|\boldsymbol{k})$.

Solution method for systems of linear equations: *Gauß-Jordan algorithm*.
Key concepts: (reduced) row-echelon form, pivot, row equivalence.

Augmented matrix and Gauß-Jordan algorithm

Solve the linear system $x + 2y = 9$, $x - 2y = -3$.

$$\begin{pmatrix} x+2y \\ x-2y \end{pmatrix} = \begin{pmatrix} 1 & 2 \\ 1 & -2 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}, \text{ thus } \boldsymbol{u} = \begin{pmatrix} x \\ y \end{pmatrix}, \mathbf{C} = \begin{pmatrix} 1 & 2 \\ 1 & -2 \end{pmatrix}, \boldsymbol{k} = \begin{pmatrix} 9 \\ -3 \end{pmatrix}.$$

$$\left(\begin{array}{rr|r} 1 & 2 & 9 \\ 1 & -2 & -3 \end{array}\right) \sim \left(\begin{array}{rr|r} 1 & 2 & 9 \\ 0 & -4 & -12 \end{array}\right) \sim \left(\begin{array}{rr|r} 1 & 2 & 9 \\ 0 & 1 & 3 \end{array}\right) \sim \left(\begin{array}{rr|r} 1 & 0 & 3 \\ 0 & 1 & 3 \end{array}\right).$$

General solution of linear systems

A system of linear equations $\mathbf{C}\boldsymbol{u} = \boldsymbol{k}$ is called

- *consistent* if it has a solution (either one or infinitely many), otherwise inconsistent (no solution at all);
- *homogeneous*[4] if the vector $\boldsymbol{k}$ on the right-hand side is zero ($\mathbf{C}\boldsymbol{u} = \mathbf{0}$), otherwise non-homogeneous or inhomogeneous.

The *nullspace (kernel)* of a matrix $\mathbf{C}$ is a linear subspace[5] formed by the solutions $\boldsymbol{u}$ of the homogeneous system $\mathbf{C}\boldsymbol{u} = \mathbf{0}$.

The *general solution $\mathcal{S}_{inh}$ of a consistent inhomogeneous linear system* $\mathbf{C}\boldsymbol{u} = \boldsymbol{k}$ is given by $\mathcal{S}_{inh} = \boldsymbol{u}_{inh} + \mathcal{S}_{hom}$ where

- $\boldsymbol{u}_{inh}$ is a *particular solution*, i.e., an arbitrary solution of the inhomogeneous system $\mathbf{C}\boldsymbol{u} = \boldsymbol{k}$, and
- $\mathcal{S}_{hom}$ is the *nullspace of* $\mathbf{C}$, i.e., the general solution of the homogeneous system $\mathbf{C}\boldsymbol{u} = \mathbf{0}$[6].

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[4] Homogeneous systems are always consistent because $\mathbf{0}$ is a solution.

[5] Note that $\mathbf{C}\{a_1\boldsymbol{u}_1 + a_2\boldsymbol{u}_2\} \;=\; a_1\mathbf{C}\boldsymbol{u}_1 + a_2\mathbf{C}\boldsymbol{u}_2 \;=\; a_1\mathbf{0} + a_2\mathbf{0} \;=\; \mathbf{0}$.

[6] If $\mathbf{C}\boldsymbol{u}_1 = \boldsymbol{k}$ and $\mathbf{C}\boldsymbol{u}_2 = \boldsymbol{k}$, then $\mathbf{C}\{\boldsymbol{u}_1 - \boldsymbol{u}_2\} \;=\; \mathbf{C}\boldsymbol{u}_1 - \mathbf{C}\boldsymbol{u}_2 \;=\; \boldsymbol{k} - \boldsymbol{k} \;=\; \mathbf{0}$.

Square matrices, identity, inverse, orthogonal matrices

A *square matrix* of order n has the same number n of rows and columns.

- A special square matrix is the *identity matrix* $\mathbf{E}$ with elements $E_{jj} = 1$ (on the diagonal) and $E_{jk} = 0$ for $j \neq k$ (outside the diagonal).
- Suppose for a square matrix $\mathbf{A}$ we can find a square matrix $\mathbf{B}$ so that $\mathbf{BA} = \mathbf{AB} = \mathbf{E}$. There is at most one such matrix $\mathbf{B}$. Then $\mathbf{A}$ is an *invertible* matrix, and $\mathbf{A}^{-1} = \mathbf{B}$ is called the *inverse of* $\mathbf{A}$.
- A system of linear equations $\mathbf{C}\boldsymbol{u} = \boldsymbol{k}$ with a square coefficient matrix $\mathbf{C}$ has a unique solution $\boldsymbol{u}$ if $\mathbf{C}$ is invertible: $\boldsymbol{u} = \mathbf{C}^{-1}\boldsymbol{k}$.

Orthogonal matrices

A real $n \times n$ matrix $\mathbf{U}$ is called an *orthogonal matrix* if its column vectors are mutually orthogonal and have unit length, so that

$$\mathbf{U}^\mathsf{T}\mathbf{U} \;=\; \mathbf{E}\,.$$

Transposition gives the inverse matrix $\mathbf{U}^{-1} \;=\; \mathbf{U}^\mathsf{T}$, thus $\mathbf{U}\mathbf{U}^\mathsf{T} = \mathbf{E}$ and also the row vectors of $\mathbf{U}$ are mutually orthogonal and have unit length.

Determinant

Invertible matrices are also called *non-singular*. A matrix that has no inverse is called *singular*. A square matrix **A** of order n is non-singular if any of the following conditions is satisfied.

- The reduced row-echelon form of the square matrix **A** is non-singular, i.e., the $(n \times n)$ RREF matrix must not have any zero rows.
- The equation $\mathbf{A}\boldsymbol{x} = \mathbf{0}$ has only the trivial solution $\boldsymbol{x} = \mathbf{0}$.
- The *determinant* of the matrix **A** *is not zero*: $\det(\mathbf{A}) \neq 0$.

Cofactor expansion of the determinant along the j-th row:

$$\det(\mathbf{A}) \;=\; \sum_{k=1}^{n} (-1)^{j+k} A_{jk} \det(\mathbf{A}_{jk}) \ .$$

Here j is the index of a specific row, A_{jk} is element in position (j,k),

- $\mathbf{A}_{jk}$ is the square matrix of order $(n-1)$ that one obtains when the j-th row and the k-th column are eliminated from **A**,
- $(-1)^{j+k} \det(\mathbf{A}_{jk})$ is the associated *cofactor*.

Eigenvalues and eigenvectors: definitions and examples

Suppose $\mathbf{A}$ is a square matrix and λ is a scalar. If a vector $\boldsymbol{v} \neq \mathbf{0}$ exists such that

$$\mathbf{A}\boldsymbol{v} \;=\; \lambda\boldsymbol{v} \;,$$

then λ is an *eigenvalue* of $\mathbf{A}$ with *eigenvector* $\boldsymbol{v}$.

- An eigenvector of unit length is also called an *invariant direction*.
- The linear subspace formed by all eigenvectors to an eigenvalue λ is called the *eigenspace* $\mathcal{E}_\lambda = \mathrm{Eig}_\lambda(\mathbf{A})$.

Real eigenvalues and eigenvectors of a real 2×2 matrix

For the matrix $\mathbf{A} = \begin{pmatrix} 1 & 4 \\ 2 & 3 \end{pmatrix}$, verify that $\boldsymbol{v}_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and $\boldsymbol{v}_2 = \begin{pmatrix} 2 \\ -1 \end{pmatrix}$ are eigenvectors, and find the corresponding eigenvalues λ_1 and λ_2.

$\mathbf{A}\boldsymbol{v}_1 = \begin{pmatrix} 1 & 4 \\ 2 & 3 \end{pmatrix}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 5 \\ 5 \end{pmatrix} = 5\boldsymbol{v}_1$, hence the eigenvalue is $\lambda_1 = 5$.

$\mathbf{A}\boldsymbol{v}_2 = -\boldsymbol{v}_2$. Eigenvalue: $\lambda_2 = -1$.

More examples of eigenvalues and eigenvectors

Not all real matrices have real eigenvalues.

Complex eigenvalues and eigenvectors of a real 2×2 matrix

For $\mathbf{A} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$, verify that $\boldsymbol{v}_1 = \begin{pmatrix} 1 \\ -\mathrm{i} \end{pmatrix}$ and $\boldsymbol{v}_2 = \begin{pmatrix} -\mathrm{i} \\ 1 \end{pmatrix}$ are eigenvectors, and find the corresponding eigenvalues λ_1 and λ_2.

$\mathbf{A}\boldsymbol{v}_1 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ -\mathrm{i} \end{pmatrix} = \begin{pmatrix} \mathrm{i} \\ 1 \end{pmatrix} = \mathrm{i}\boldsymbol{v}_1$, hence the eigenvalue is $\lambda_1 = \mathrm{i}$.

$\mathbf{A}\boldsymbol{v}_2 = -\mathrm{i}\boldsymbol{v}_2$. Eigenvalue: $\lambda_2 = -\mathrm{i}$.

Remarks

- *Singular matrices*: kernel is the eigenspace $\mathcal{E}_0$ to the eigenvalue $\lambda = 0$.
- *Identity* (map/matrix): eigenvalue $\lambda = 1$, all vectors are eigenvectors.
- *Diagonal matrices* $\mathbf{D} = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$: diagonal elements λ_j are eigenvalues, standard basis vectors $\hat{\boldsymbol{e}}_j$ are eigenvectors.

How to find the eigenvalues of a (small) matrix

The eigenvalue-eigenvector equation $\mathbf{A}\boldsymbol{v} = \lambda\boldsymbol{v}$ for a square matrix $\mathbf{A}$ can be rearranged to yield $(\lambda\mathbf{E} - \mathbf{A})\boldsymbol{v} = \mathbf{0}$. This implies that a non-zero eigenvector must be in the kernel of the operator $\lambda\mathbf{E} - \mathbf{A}$, and

$$P_{\mathbf{A}}(\lambda) \;=\; \det(\lambda\mathbf{E} - \mathbf{A}) \;=\; 0\;.$$

The eigenvalues of $\mathbf{A}$ are the roots of the function $P_{\mathbf{A}}(\lambda) = \det(\lambda\mathbf{E} - \mathbf{A})$, the so-called *characteristic polynomial of* $\mathbf{A}$.

Characteristic polynomial of a real 2×2 matrix

Find the eigenvalues of the matrix $\mathbf{A} = \begin{pmatrix} 0 & -1 \\ 2 & 3 \end{pmatrix}$.

Characteristic polynomial: $P_{\mathbf{A}}(\lambda) \;=\; \det\begin{pmatrix} \lambda & 1 \\ -2 & \lambda - 3 \end{pmatrix} \;=\; \lambda^2 - 3\lambda + 2,$

thus $P_{\mathbf{A}}(\lambda) \;=\; (\lambda - 1)\cdot(\lambda - 2)$. The eigenvalues are $\lambda = 1$ and $\lambda = 2$.

How to find the eigenvectors of a (small) matrix

Gauß-Jordan algorithm

Suppose λ is an eigenvalue of the matrix **A**. To find an eigenvector $\boldsymbol{v}$,

- construct the matrix $(\mathbf{A} - \lambda\mathbf{E})$,
- apply a series of elementary row operations to
- yield a row-equivalent form with only zeros in the last row, then
- obtain an eigenvector $\boldsymbol{v}$ by backsubstitution.

Computing the eigenvector of a real 3×3 matrix

For $\mathbf{A} = \begin{pmatrix} 33 & -12 & 0 \\ -12 & 27 & 12 \\ 0 & 12 & 21 \end{pmatrix}$ and the eigenvalue $\lambda = 9$ find an eigenvector.

$$\begin{pmatrix} 24 & -12 & 0 \\ -12 & 18 & 12 \\ 0 & 12 & 12 \end{pmatrix} \sim \begin{pmatrix} 24 & -12 & 0 \\ 0 & 12 & 12 \\ 0 & 12 & 12 \end{pmatrix} \sim \begin{pmatrix} 1 & 0 & \frac{1}{2} \\ 0 & 1 & 1 \\ 0 & 0 & 0 \end{pmatrix}$$

Set $v_3 = 2$, then $v_2 = -2$ and $v_1 = -1$, thus $\boldsymbol{v} = (-1, -2, 2)^\mathsf{T}$ and $\hat{\boldsymbol{v}} = \boldsymbol{v}/|\boldsymbol{v}| = \boldsymbol{v}/3$.

Numerical methods, diagonalization of matrices

Numerical methods: Finding eigenvalues and eigenvectors of large matrices with the method outlined above (characteristic polynomial, Gauß-Jordan algorithm) can become computationally expensive and even numerically unstable. Instead, iterative methods such as QR decomposition (with an initial Householder transformation to a Hessenberg matrix) are used to transform the matrix to an equivalent form from which eigenvalues and eigenvalues are efficiently obtained.

Diagonalization of matrices

A $n \times n$ matrix $\mathbf{A}$ is said to be *diagonalizable* over $\mathbb{R}$ (or over $\mathbb{C}$) if a basis of $\mathbb{R}^n$ (or $\mathbb{C}^n$) can be constructed from the eigenvectors of $\mathbf{A}$.

- When these basis vectors form the columns of a matrix $\mathbf{T}$, then $\mathbf{D} = \mathbf{T}^{-1}\mathbf{A}\mathbf{T}$ is a diagonal matrix of eigenvalues, and $\mathbf{A} = \mathbf{T}\mathbf{D}\mathbf{T}^{-1}$.
- The process of finding such a decomposition is called *diagonalization*.
- A $n \times n$ matrix can be diagonalized if it has n distinct eigenvalues (sufficient condition, not necessary).

Symmetric matrices

A matrix $\mathbf{A}$ is called *symmetric* if it equals its own transpose: $\mathbf{A} = \mathbf{A}^{\mathsf{T}}$.

For any real symmetric $n \times n$ matrix $\mathbf{A}$,

- the eigenvalues are all real,
- an orthonormal basis of $\mathbb{R}^n$ can be constructed from its eigenvectors,
- a real diagonal matrix $\mathbf{D}$ and an orthogonal transformation matrix $\mathbf{T}$ exist such that $\mathbf{A} = \mathbf{T}\mathbf{D}\mathbf{T}^{\mathsf{T}}$.

Diagonal matrix $\mathbf{D}$ for a real symmetric 3×3 matrix $\mathbf{A}$

$\mathbf{A} = \begin{pmatrix} 33 & -12 & 0 \\ -12 & 27 & 12 \\ 0 & 12 & 21 \end{pmatrix}$, $\mathbf{T} = \frac{1}{3}\begin{pmatrix} 1 & 2 & 2 \\ 2 & 1 & -2 \\ -2 & 2 & -1 \end{pmatrix}$. Compute $\mathbf{T}^{\mathsf{T}}\mathbf{T}$ and $\mathbf{T}^{\mathsf{T}}\mathbf{A}\mathbf{T}$.

$$\mathbf{T}^{\mathsf{T}}\mathbf{T} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad \mathbf{T}^{\mathsf{T}}\mathbf{A}\mathbf{T} = \begin{pmatrix} 9 & 0 & 0 \\ 0 & 27 & 0 \\ 0 & 0 & 45 \end{pmatrix} = \mathbf{D}\ .$$

Dyadic representation: $\mathbf{A} = \sum_j \lambda_j \hat{\boldsymbol{v}}_j \hat{\boldsymbol{v}}_j^{\mathsf{T}} = \sum_j \lambda_j |\hat{\boldsymbol{v}}_j\rangle\langle\hat{\boldsymbol{v}}_j|\ .$

Eigenvalues and eigenvectors

Consider $\mathbf{M} = \begin{pmatrix} 5 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 5 \end{pmatrix}$, $\boldsymbol{v}_1 = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}$, and $\boldsymbol{v}_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$.
Show that $\boldsymbol{v}_1$ and $\boldsymbol{v}_2$ are eigenvectors of $\mathbf{M}$. Compute the corresponding eigenvalues λ_1 and λ_2. Construct an independent eigenvector and find the eigenvalue λ_3. Verify $\mathbf{M} = \sum_\ell \lambda_\ell \hat{\boldsymbol{v}}_\ell \hat{\boldsymbol{v}}_\ell^\mathsf{T}$.

$\mathbf{M}\boldsymbol{v}_1 = \begin{pmatrix} 5 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 5 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 6 \\ 0 \\ 6 \end{pmatrix} = 6 \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}$, thus $\boldsymbol{v}_1$ is an eigenvector of $\mathbf{M}$ with eigenvalue $\lambda_1 = 6$.

$\mathbf{M}\boldsymbol{v}_2 = \begin{pmatrix} 5 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 5 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 2 \\ 0 \end{pmatrix} = 2 \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$, thus $\boldsymbol{v}_2$ is an eigenvector of $\mathbf{M}$ with eigenvalue $\lambda_2 = 2$.

The vector $\boldsymbol{v}_3 = \boldsymbol{v}_1 \times \boldsymbol{v}_2 = (-1, 0, 1)^\mathsf{T}$ is orthogonal to both $\boldsymbol{v}_1$ and $\boldsymbol{v}_2$. Since $\mathbf{M}$ is symmetric, $\boldsymbol{v}_3$ is also an eigenvector. This can be verified by evaluating $\mathbf{M}\boldsymbol{v}_3 = 4\boldsymbol{v}_3$, thus $\boldsymbol{v}_3$ is an eigenvector of $\mathbf{M}$ with eigenvalue $\lambda_3 = 4$.

Normalizing the vectors $\boldsymbol{v}_1$, $\boldsymbol{v}_2$, $\boldsymbol{v}_3$ yields $\hat{\boldsymbol{v}}_1 = \left(\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right)^\mathsf{T}$, $\hat{\boldsymbol{v}}_2 = (0, 1, 0)^\mathsf{T}$, $\hat{\boldsymbol{v}}_3 = \left(-\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right)^\mathsf{T}$.

The three dyads $\hat{\boldsymbol{v}}_\ell \hat{\boldsymbol{v}}_\ell^\mathsf{T}$ are $\hat{\boldsymbol{v}}_1 \hat{\boldsymbol{v}}_1^\mathsf{T} = \begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}$, $\hat{\boldsymbol{v}}_2 \hat{\boldsymbol{v}}_2^\mathsf{T} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$, $\hat{\boldsymbol{v}}_3 \hat{\boldsymbol{v}}_3^\mathsf{T} = \begin{pmatrix} \frac{1}{2} & 0 & -\frac{1}{2} \\ 0 & 0 & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}$,
thus $\sum_\ell \lambda_\ell \hat{\boldsymbol{v}}_\ell \hat{\boldsymbol{v}}_\ell^\mathsf{T} = \begin{pmatrix} 3 & 0 & 3 \\ 0 & 0 & 0 \\ 3 & 0 & 3 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 2 & 0 & -2 \\ 0 & 0 & 0 \\ -2 & 0 & 2 \end{pmatrix} = \begin{pmatrix} 5 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 5 \end{pmatrix} = \mathbf{M}$.

Singular value decomposition of a rectangular matrix

Singular value decomposition (SVD) of a rectangular $N \times L$ matrix $\mathbf{M}$:

$$\mathbf{M} \ = \ \mathbf{U}\,\mathbf{S}\,\mathbf{V}^{\mathsf{T}} \ .$$

- $\mathbf{V}$ is an orthogonal $L \times L$ matrix with column vectors $\hat{\boldsymbol{v}}_\ell$.
- $\mathbf{S} = \mathrm{diag}(s_1, s_2, \ldots, s_L)$ is the diagonal matrix of *singular values* arranged in descending order: $s_1 \geq s_2 \geq \ldots \geq s_L \geq 0$.
- $\mathbf{U}$ is a $N \times L$ matrix that is column orthogonal ($\mathbf{U}^{\mathsf{T}}\mathbf{U} = \mathbf{1}$). The column vectors $\hat{\boldsymbol{u}}_\ell$ of $\mathbf{U}$ are orthonormal.

Singular values and eigenvalues

Given the SVD of $\mathbf{M}$, compute eigenvalues and eigenvectors of $\mathbf{M}^{\mathsf{T}}\mathbf{M}$.

Using the identity $(\mathbf{A}\mathbf{B})^{\mathsf{T}} = \mathbf{B}^{\mathsf{T}}\mathbf{A}^{\mathsf{T}}$, we write $\left(\mathbf{U}\,\mathbf{S}\,\mathbf{V}^{\mathsf{T}}\right)^{\mathsf{T}} = \mathbf{V}\,\mathbf{S}^{\mathsf{T}}\mathbf{U}^{\mathsf{T}}$ and

$$\mathbf{M}^{\mathsf{T}}\mathbf{M} \ = \ \mathbf{V}\,\mathbf{S}^{\mathsf{T}}\mathbf{U}^{\mathsf{T}}\mathbf{U}\,\mathbf{S}\,\mathbf{V}^{\mathsf{T}} \ = \ \mathbf{V}\,\mathbf{S}^{\mathsf{T}}\mathbf{S}\,\mathbf{V}^{\mathsf{T}} \ = \ \mathbf{V}\,\mathbf{S}^2\,\mathbf{V}^{\mathsf{T}} \ .$$

Thus $\mathbf{M}^{\mathsf{T}}\mathbf{M}$ has eigenvalues $\gamma_\ell = s_\ell^2$ and eigenvectors $\hat{\boldsymbol{v}}_\ell$.

Sample problems

Singular value decomposition

Consider the matrices $\mathbf{M} = \begin{pmatrix} -12 & 9 \\ 150 & 200 \\ 16 & -12 \end{pmatrix}$ and $\mathbf{U} = \begin{pmatrix} 0 & 3/5 \\ 1 & 0 \\ 0 & -4/5 \end{pmatrix}$.

Compute $\mathbf{M}\mathbf{M}^\mathsf{T}$. Show that the column vectors of $\mathbf{U}$ are eigenvectors of $\mathbf{M}\mathbf{M}^\mathsf{T}$ with nonzero eigenvalues γ_1 and γ_2. Compute $s_1 = \sqrt{\gamma_1}$ and $s_2 = \sqrt{\gamma_2}$. Construct the matrix $\mathbf{V}$ in the SVD of $\mathbf{M} = \mathbf{U}\mathbf{S}\mathbf{V}^\mathsf{T}$.

The matrix products $\mathbf{M}\mathbf{M}^\mathsf{T}$ and $\mathbf{M}\mathbf{M}^\mathsf{T}\mathbf{U}$ are

$$\mathbf{M}\mathbf{M}^\mathsf{T} = \begin{pmatrix} 225 & 0 & -300 \\ 0 & 62500 & 0 \\ -300 & 0 & 400 \end{pmatrix} \quad \Rightarrow \quad \mathbf{M}\mathbf{M}^\mathsf{T}\mathbf{U} = \begin{pmatrix} 0 & 375 \\ 62500 & 0 \\ 0 & -500 \end{pmatrix} .$$

The first column vector of $\mathbf{U}$ is an eigenvector with eigenvalue $\gamma_1 = 62500$, and the second column vector is an eigenvector with eigenvalue $\gamma_2 = 625$. The corresponding singular values of $\mathbf{M}$ are $s_1 = 250$ and $s_2 = 25$.

Rearranging $\mathbf{M} = \mathbf{U}\mathbf{S}\mathbf{V}^\mathsf{T}$ gives $\mathbf{V} = \left(\mathbf{S}^{-1}\mathbf{U}^\mathsf{T}\mathbf{M}\right)^\mathsf{T} = \begin{pmatrix} 3/5 & -4/5 \\ 4/5 & 3/5 \end{pmatrix}$.

Numerical Software Lab

NumPy arrays

- Array definitions, shape, elementwise array operations.

Matrix operations in NumPy

- Matrix products: `dot()`, `matmul()`.
- Systems of linear equations: `linalg.solve()`
- Matrix inverse and determinant: `linalg.inv()`, `linalg.det()`
- Exercises

Matrix decompositions

- Eigenvalues: `linalg.eig()`
- Singular values: `linalg.svd()`
- Exercises

Data modeling and numerical linear algebra

Terminology in data modeling

Statistical modeling of data: assume the observed data d result from a deterministic model m and a random component r (noise).

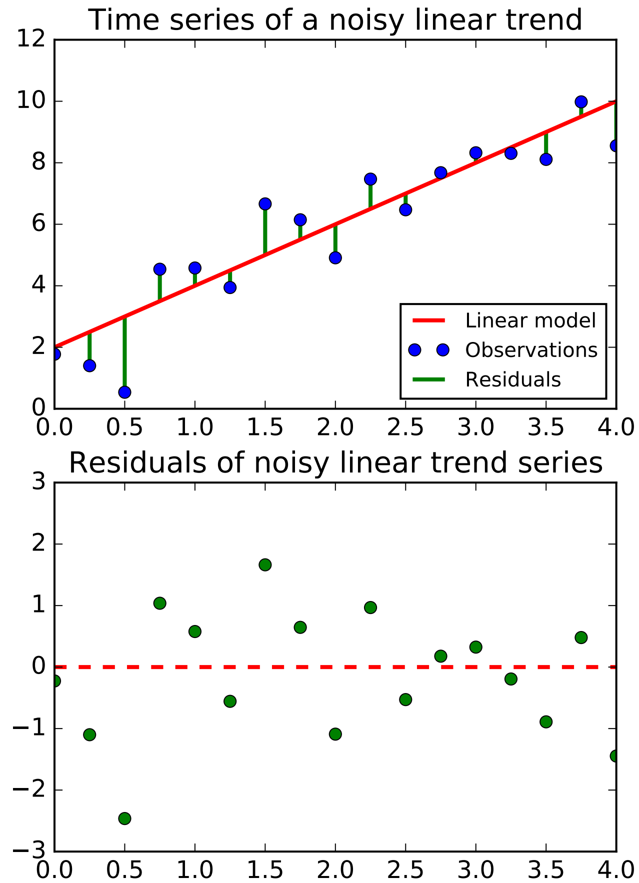
Independent variable t (time): d_t, $d(t)$, m_t, ...

In model equations of the type $d_t = m_t + r_t$ or $d(t) = m(t) + r(t)$,

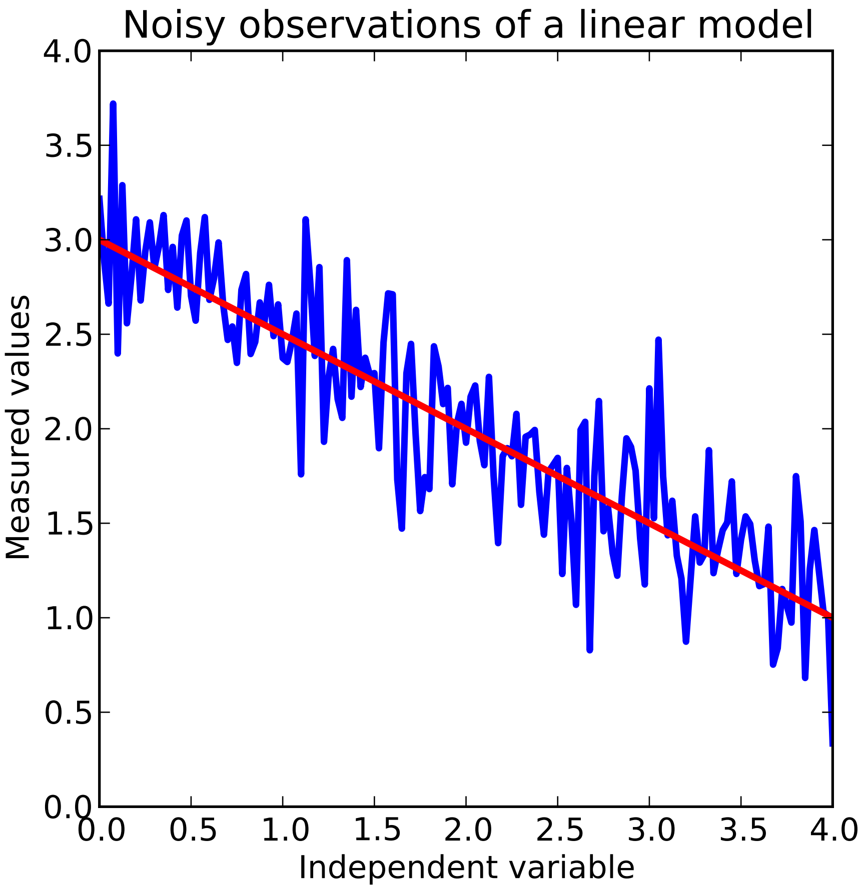
- the model function $m_t = m(t)$ is often referred to as *prediction*, and
- the noise term $r_t = d_t - m_t$ may also be called *residual* or error.

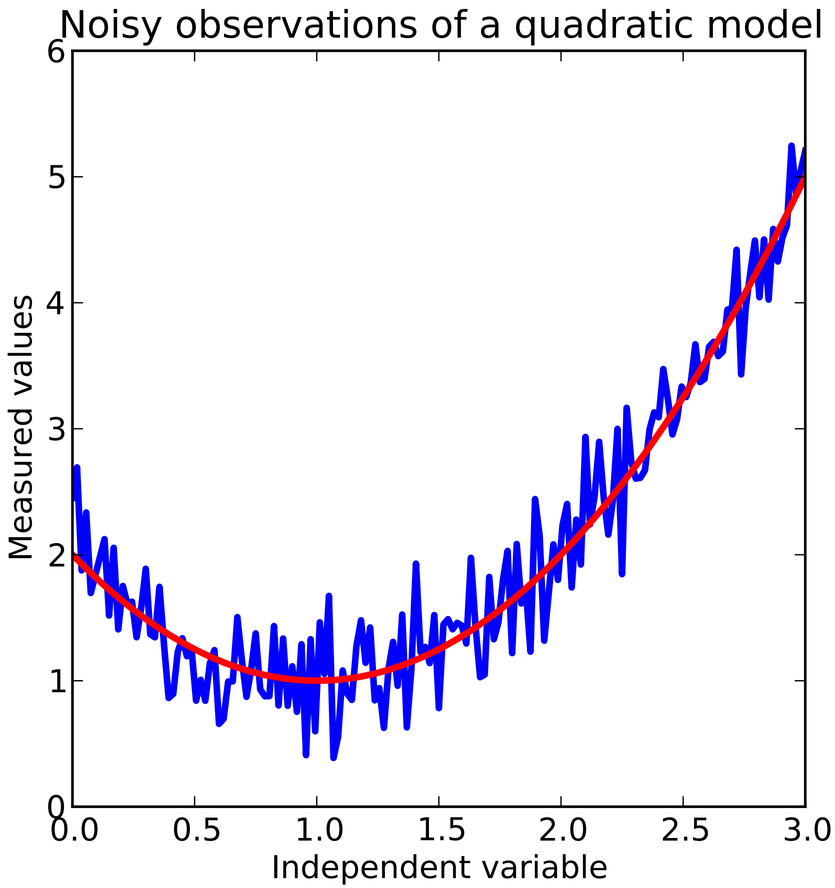
The prediction $m(t)$ usually depends on one or more *model parameters* $\boldsymbol{\omega}$. We write $m(t|\boldsymbol{\omega})$ to make this dependence explicit.

E.g., linear trend: $m(t|a, b) = a + bt$.



Models that are linear in the parameters

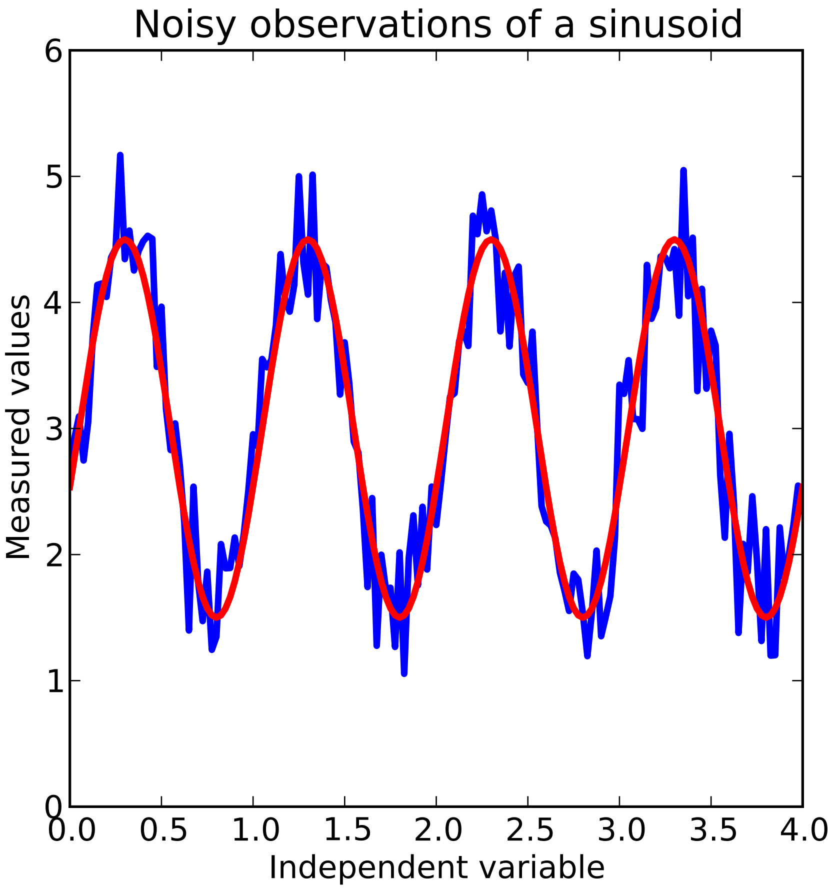


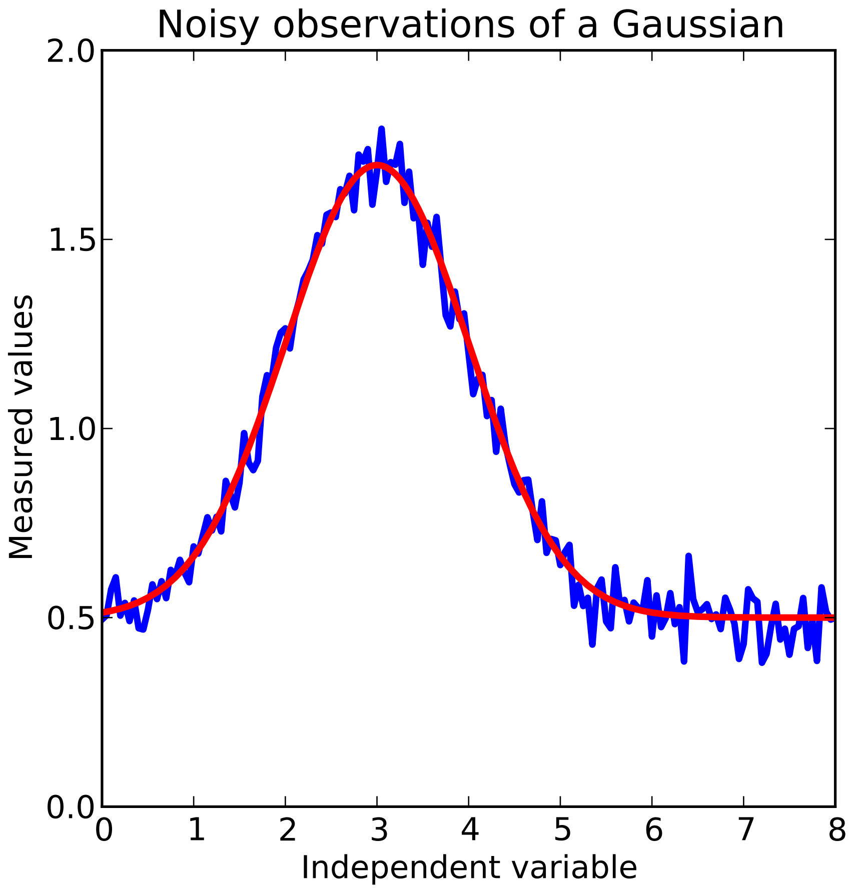


$$m(t|a_1, a_2) = a_1 + a_2 \cdot t$$

$$m(t|a_1, a_2, a_3) = a_1 + a_2 \cdot t + a_3 \cdot t^2$$

Models that are nonlinear in some parameters





$$m(t|a_1, a_2, \omega, \phi) = a_1 + a_2 \cdot \cos(\omega t + \phi)$$

$$m(x|a_1, a_2, \mu, \sigma^2) = a_1 + a_2 \cdot \exp\left\{-(x-\mu)^2/2\sigma^2\right\}$$

Parameter estimation strategies

Parameter estimation can be based on different optimality criteria.

- Maximize the (data) likelihood $\mathrm{P}(d|m,\boldsymbol{\omega})$: probability distribution needs to be known for *maximum-likelihood (ML) estimation*.
- Minimize the *absolute deviation* $\sum_t |d(t) - m(t|\boldsymbol{\omega})|$: robust class of estimators but only few analytical results.
- Minimize $\chi^2 \propto \sum_t [d(t) - m(t|\boldsymbol{\omega})]^2$ to yield a *least squares estimator*: well understood and many analytical results but less robust.

If the measurement errors $r_t = d_t - m_t$ form an i.i.d. sample drawn from a *normal distribution* $p(r_t|\boldsymbol{\omega}) \propto \exp\{-r_t^2/2\sigma^2\}$, maximizing the likelihood is equivalent to minimizing $\sum_t r_t^2/2\sigma^2 \propto \sum_t (d_t - m_t)^2$, i.e., the least squares approach.

When the uncertainty of individual measurements is not independent of t, then $\sigma \to \sigma_t$ and the *least squares condition* becomes

$$\chi^2 = \sum_t \left(\frac{d(t) - m(t|\boldsymbol{\omega})}{\sigma_t} \right)^2 \stackrel{!}{=} \text{Min} .$$

Matrix formulation of linear parameter estimation problems

Models that are *linear in all parameters* can be written in the form

$$m(t) \;=\; \sum_{\ell=1}^{L} a_\ell f_\ell(t)$$

where f_ℓ are given functions of the independent variable called the *basis functions*. The parameters $a_1, a_2, \ldots, a_L$ can be understood as amplitudes.

When N measurements d_n are supposed to be modeled, the conditions $m(t_n) = d_n$ yield a *linear system* $\mathbf{M}\boldsymbol{a} \;=\; \boldsymbol{d}$ where

- $\mathbf{M}$ is the $N \times L$ *design matrix* with elements $M_{n\ell} = f_\ell(t_n)$,
- $\boldsymbol{a} = (a_1, a_2, \ldots, a_L)^\mathsf{T}$ is the vector of L *model parameters*,
- $\boldsymbol{d} = (d_1, d_2, \ldots, d_N)^\mathsf{T}$ comprises N *measured values*.

In the presence of possibly different *measurement errors* σ_n, the model matrix and the data vector should be properly scaled:

$$f_\ell(t_n) \;\rightarrow\; \frac{f_\ell(t_n)}{\sigma_n} \quad \text{and} \quad d_n \;\rightarrow\; \frac{d_n}{\sigma_n} \;.$$

Solution space of linear systems

Suppose the $N \times L$ matrix $\mathbf{M}$ has *full rank* $= \min(N, L)$. Then the linear system of equations $\mathbf{M}\boldsymbol{a} = \boldsymbol{d}$, i.e.,

$$\begin{pmatrix} M_{11} & M_{12} & \cdots & M_{1L} \\ M_{21} & M_{22} & \cdots & M_{2L} \\ M_{31} & M_{32} & \cdots & M_{3L} \\ M_{41} & M_{42} & \cdots & M_{4L} \\ \vdots & \vdots & \vdots & \vdots \\ M_{N1} & M_{N2} & \cdots & M_{NL} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_L \end{pmatrix} = \begin{pmatrix} d_1 \\ d_2 \\ d_3 \\ d_4 \\ \vdots \\ d_N \end{pmatrix},$$

is called

- *overdetermined* if $N > L$ (more constraints than unknowns),
- *underdetermined* if $N < L$ (less constraints than unknowns),
- *equidetermined* if $N = L$.

In a *strict formal sense*, an

- overdetermined system has no solution at all,
- underdetermined system has many solutions,
- equidetermined system has a unique solution.

Example, inverse matrix

Polynomial fitting as a parameter estimation problem

Consider straight line fitting. When do you expect the parameter estimation problem to be underdetermined, overdetermined, equidetermined ? How about fitting a polynomial of degree D ?

A straight line is described by $L = 2$ parameters.

- One point, $N = 1$: underdetermined (infinitely many straight lines).
- Two points ($N = 2$): equidetermined (exactly on straight line).
- Three or more points ($N \geq 3$): overdetermined (in general, no straight line can be found that passes through all given points).

Polynomial, degree D: equidetermined when $N = D + 1$ points are given.

In the equidetermined case $N = L$ (square matrix), the full rank condition implies that $\mathbf{M}$ is a *non-singular* matrix with *inverse* $\mathbf{M}^{-1}$. The solution of the linear system $\mathbf{M}\boldsymbol{a} = \boldsymbol{d}$ can then formally be written as

$$\boldsymbol{a} = \mathbf{M}^{-1}\boldsymbol{d} \, .$$

Classroom exercise

A simple ill-conditioned problem

Suppose $N = L = 2$ with the matrix $\mathbf{M} = \begin{pmatrix} 101 & 99 \\ 99 & 101 \end{pmatrix}$. Measurements are $d_1 = d_2 = 200$. Compute the parameter vector $\boldsymbol{a}$. Assuming an uncertainty of 5%, compute the solution also for $d_1 = 210$ and $d_2 = 190$.

The inverse is $\mathbf{M}^{-1} = \dfrac{1}{400} \begin{pmatrix} 101 & -99 \\ -99 & 101 \end{pmatrix}$.

$$\boldsymbol{d} = \begin{pmatrix} 200 \\ 200 \end{pmatrix} \quad \Rightarrow \quad \boldsymbol{a} = \mathbf{M}^{-1}\boldsymbol{d} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} .$$

$$\boldsymbol{d} = \begin{pmatrix} 210 \\ 190 \end{pmatrix} \quad \Rightarrow \quad \boldsymbol{a} = \mathbf{M}^{-1}\boldsymbol{d} = \begin{pmatrix} 6 \\ -4 \end{pmatrix} .$$

Here a 5% uncertainty in the measured values yields deviations in the estimated parameters of 500%, i.e., errors are amplified by a factor of 100.

Condition number

When small uncertainties in the data can yield large variations in the estimated parameters, the problem is said to be *ill-conditioned*. The maximum error amplification factor is the *condition number*

$$\kappa(\mathbf{M}) \;=\; \mathrm{cond}(\mathbf{M}) \;=\; \|\mathbf{M}\| \cdot \|\mathbf{M}^{-1}\|$$

where $\| \bullet \|$ is an appropriate matrix norm. For the 2-norm, the condition number is the ratio of largest to smallest singular values.

Square matrices: ratio of largest to smallest eigenvalue magnitudes.

Condition number example

Compute the eigenvalues and the condition number of $\mathbf{M} = \begin{pmatrix} 101 & 99 \\ 99 & 101 \end{pmatrix}$.

The eigenvalues are $\lambda_1 = 200$ and $\lambda_2 = 2$. The condition number is $\kappa = 100$. Eigenvectors (non-normalized) are $\boldsymbol{a}_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and $\boldsymbol{a}_2 = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$.

Generalized inverses

Linear systems $\mathbf{M}\boldsymbol{a} = \boldsymbol{d}$ do not have unique solutions $\boldsymbol{a}$ when the $(N \times L)$ matrix $\mathbf{M}$ is rectangular (non-square, $N \neq L$). *Generalized inverses* or *pseudo-inverses* for rectangular matrices can be defined as follows.

Overdetermined case $(N > L)$. The vector $\boldsymbol{a}$ that minimizes the square deviation $|\boldsymbol{r}|^2 = |\mathbf{M}\boldsymbol{a} - \boldsymbol{d}|^2$ is given by

$$\boldsymbol{a} \;=\; \left(\mathbf{M}^{\mathsf{T}}\mathbf{M}\right)^{-1}\mathbf{M}^{\mathsf{T}}\boldsymbol{d} \;=\; \mathbf{M}^{\mathrm{ils}}\boldsymbol{d} \quad \text{with} \quad \mathbf{M}^{\mathrm{ils}} \;=\; \left(\mathbf{M}^{\mathsf{T}}\mathbf{M}\right)^{-1}\mathbf{M}^{\mathsf{T}} \,.$$

The matrix $\mathbf{M}^{\mathrm{ils}}$ is the pseudo-inverse in the least-squares sense.

Underdetermined case $(N < L)$. From the space of all possible solutions we select the shortest vector $\boldsymbol{a}$ by minimizing the (square) norm $|\boldsymbol{a}|^2$ subject to $\mathbf{M}\boldsymbol{a} = \boldsymbol{d}$ (Lagrange multiplier technique). We find

$$\boldsymbol{a} \;=\; \mathbf{M}^{\mathsf{T}}\left(\mathbf{M}\mathbf{M}^{\mathsf{T}}\right)^{-1}\boldsymbol{d} \;=\; \mathbf{M}^{\mathrm{imn}}\boldsymbol{d} \quad \text{with} \quad \mathbf{M}^{\mathrm{imn}} \;=\; \mathbf{M}^{\mathsf{T}}\left(\mathbf{M}\mathbf{M}^{\mathsf{T}}\right)^{-1} \,.$$

The matrix $\mathbf{M}^{\mathrm{imn}}$ is the pseudo-inverse in this (minimum norm) case.

Sample problems

Straight line fitting: design matrix

In straight line fitting, the model function is $m(t) = a_1 + a_2 t$. Suppose three measurements are taken at t_1, t_2, t_3 that yield data d_1, d_2, d_3 with identical errors: $\sigma_n = \sigma$. Find the design matrix $\mathbf{M}$ and compute $\mathbf{M}^\mathsf{T}\mathbf{M}$ for the following two cases.

(a) $t_1 = -1, t_2 = 0, t_3 = 1.$

(b) $t_1 = 1, t_2 = 2, t_3 = 3.$

The two basis functions are $f_1(t) = 1$ and $f_2(t) = t$. The elements of the design matrix $\mathbf{M}$ are

- $M_{n1} = \dfrac{f_1(t_n)}{\sigma} = \dfrac{1}{\sigma}$ and
- $M_{n2} = \dfrac{f_2(t_n)}{\sigma} = \dfrac{t_n}{\sigma}$

for $n = 1, 2, 3$.

(a) $\mathbf{M} = \sigma^{-1}\begin{pmatrix} 1 & -1 \\ 1 & 0 \\ 1 & 1 \end{pmatrix}$, $\mathbf{M}^\mathsf{T}\mathbf{M} = \sigma^{-2}\begin{pmatrix} 3 & 0 \\ 0 & 2 \end{pmatrix}$.

(b) $\mathbf{M} = \sigma^{-1}\begin{pmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{pmatrix}$, $\mathbf{M}^\mathsf{T}\mathbf{M} = \sigma^{-2}\begin{pmatrix} 3 & 6 \\ 6 & 14 \end{pmatrix}$.

Stability of matrix inversion

In practice, parameter estimation problems may be both

- overdetermined (less unknowns than noisy data) and
- ill-conditioned (sensitivity to measurement errors),

so we need means to *stabilize matrix inversion*.

Consider the overdetermined case: $\left(\mathbf{M}^\mathsf{T}\mathbf{M}\right)^{-1}$. Using its L eigenvalues γ_ℓ (all non-negative), the symmetric $L \times L$ matrix $\mathbf{M}^\mathsf{T}\mathbf{M}$ can be decomposed

$$\mathbf{M}^\mathsf{T}\mathbf{M} \;=\; \mathbf{V}\,\mathbf{G}\,\mathbf{V}^\mathsf{T} \;.$$

$\mathbf{V}$ is orthogonal ($\mathbf{V}^\mathsf{T}\mathbf{V} = \mathbf{V}\mathbf{V}^\mathsf{T} = \mathbf{1}$), and $\mathbf{G} = \mathrm{diag}(\gamma_1, \gamma_2, \ldots, \gamma_L)$ with the eigenvalues arranged as $\gamma_1 \geq \gamma_2 \geq \ldots \geq \gamma_L \geq 0$. The columns of $\mathbf{V}$ are normalized eigenvectors $\hat{\boldsymbol{v}}_\ell$ of $\mathbf{M}^\mathsf{T}\mathbf{M}$. We may write

$$\mathbf{M}^\mathsf{T}\mathbf{M} \;=\; \sum_{\ell=1}^{L} \gamma_\ell \hat{\boldsymbol{v}}_\ell \hat{\boldsymbol{v}}_\ell^\mathsf{T} \quad \text{and} \quad \left(\mathbf{M}^\mathsf{T}\mathbf{M}\right)^{-1} \;=\; \sum_{\ell=1}^{L} \gamma_\ell^{-1} \hat{\boldsymbol{v}}_\ell \hat{\boldsymbol{v}}_\ell^\mathsf{T} \;.$$

Unstable inversion is caused by very small eigenvalues. If $\gamma_\ell \ll \gamma_1 = \gamma_{\mathsf{max}}$ for indices $\ell > L^*$, then for a stable inversion omit these contributions: $L \to L^*$.

Sample problems

Straight line fitting: error ellipsoid

Consider the linear regression model $m(t) = a_1 + a_2 t$ with three measurements d_1, d_2, d_3 at t_1, t_2, t_3 and identical errors ($\sigma_n = \sigma$) at (a) $t_1 = -1, t_2 = 0, t_3 = 1$ and (b) $t_1 = 1, t_2 = 2, t_3 = 3$. Find the orientation of the error ellipsoid using the eigenvalue-eigenvector decomposition $\mathbf{VGV}^\mathsf{T}$ of $\mathbf{M}^\mathsf{T}\mathbf{M}$. Are the errors of the two regression parameters correlated or uncorrelated ?

The eigenvectors $\hat{\boldsymbol{v}}_1, \hat{\boldsymbol{v}}_2$ of $\mathbf{M}^\mathsf{T}\mathbf{M}$ give the orientation of the error ellipsoid. Parameter estimation errors are uncorrelated if the eigenvectors coincide with the coordinate axes, otherwise correlated. The eigenvalue ratio γ_1/γ_2 is the condition number of $\mathbf{M}^\mathsf{T}\mathbf{M}$ and thus an indicator for the stability of the matrix inversion in the normal equations.

(a) $\mathbf{M}^\mathsf{T}\mathbf{M} = \sigma^{-2}\begin{pmatrix} 3 & 0 \\ 0 & 2 \end{pmatrix}$ yields $\hat{\boldsymbol{v}}_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\hat{\boldsymbol{v}}_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. The errors are uncorrelated. Since $\gamma_1/\gamma_2 = 1.5$ is close to unity, the problem is well-conditioned, and an inversion will be stable.

(b) $\mathbf{M}^\mathsf{T}\mathbf{M} = \sigma^{-2}\begin{pmatrix} 3 & 6 \\ 6 & 14 \end{pmatrix}$ yields $\hat{\boldsymbol{v}}_1 \simeq \begin{pmatrix} 0.403 \\ 0.915 \end{pmatrix}$ and $\hat{\boldsymbol{v}}_2 \simeq \begin{pmatrix} -0.915 \\ 0.403 \end{pmatrix}$. The errors are correlated. Since $\gamma_1/\gamma_2 \simeq 16.64/0.3606 \simeq 46$, the problem is less well-conditioned than in case (a), and the matrix inversion in the solution of the normal equations will be less stable.

Stable matrix inversion using SVD

SVD allows to represent $\mathbf{M}$ as a sum of dyadic products:

$$\mathbf{M} \;=\; \mathbf{U}\,\mathbf{S}\,\mathbf{V}^{\mathsf{T}} \;=\; \sum_{\ell=1}^{L} s_\ell \hat{\boldsymbol{u}}_\ell \hat{\boldsymbol{v}}_\ell^{\mathsf{T}} \;.$$

Singular values s_ℓ that are too small compared with the maximum value s_1 cause matrix inversion to be unstable. Assuming $s_\ell \ll s_1$ for $\ell > L^*$, we define the *generalized inverse of* $\mathbf{M}$ *in the SVD sense* as

$$\mathbf{M}^{\mathsf{isv}} \;=\; \sum_{\ell=1}^{L^*} s_\ell^{-1} \hat{\boldsymbol{v}}_\ell \hat{\boldsymbol{u}}_\ell^{\mathsf{T}} \;=\; \mathbf{V}\,\mathbf{S}^{-*}\,\mathbf{U}^{\mathsf{T}}$$

where $\mathbf{S}^{-*} \;=\; \mathrm{diag}\left(s_1^{-1}, s_2^{-1}, \ldots, s_{L^*}^{-1}, 0, \ldots, 0\right)$.

Singular values, eigenvalues, and matrix inversion

Compared with the eigenvalues γ_ℓ of $\mathbf{M}^{\mathsf{T}}\mathbf{M}$, the singular values s_ℓ of $\mathbf{M}$ yield better truncation criteria for stabilizing matrix inversion. Why?

Further comments on SVD and numerical matrix inversion

SVD procedure to carry out stable matrix inversion

- *Diagnose the matrix* through its singular values, condition number, vectors $\hat{\boldsymbol{u}}_\ell$ and vectors $\hat{\boldsymbol{v}}_\ell$.
- *Identify potential instabilities* through the singular values that are too small for a reliable matrix inversion.
- *Construct the generalized inverse* using only those terms that are associated with sufficiently large singular values.

Alternative representation of SVD: $\mathbf{M} = \tilde{\mathbf{U}}\,\tilde{\mathbf{S}}\,\mathbf{V}^\mathsf{T}$. Here $\tilde{\mathbf{U}}$ is a $N \times N$ orthogonal matrix. The first L rows of the $N \times L$ matrix $\tilde{\mathbf{S}}$ are identical with the diagonal matrix $\mathbf{S}$, the remaining rows are filled with zeros.

Stable matrix inversion through *damping* or *regularization*

- Tikhonov regularization: $\left(\mathbf{M}^\mathsf{T}\mathbf{M}\right)^{-1} \rightarrow \left(\mathbf{M}^\mathsf{T}\mathbf{M} + \boldsymbol{\Gamma}^\mathsf{T}\boldsymbol{\Gamma}\right)^{-1}$.
- E.g., $\left(\mathbf{M}^\mathsf{T}\mathbf{M}\right)^{-1} \rightarrow \left(\mathbf{M}^\mathsf{T}\mathbf{M} + \lambda^2\mathbf{1}\right)^{-1}$ with a damping parameter λ.

Scaling of measurement errors and model misfits

Least squares estimators minimize the sum of error-scaled squared residuals or, equivalently, the (error-scaled) mean-square residual

$$\left\langle \left(\frac{d(t) - m(t)}{\sigma(t)} \right)^2 \right\rangle = \frac{1}{N-L} \sum_{n=1}^{N} \left(\frac{d_n - m(t_n)}{\sigma_n} \right)^2 .$$

The square root of this expression is the rms (root-mean-square) misfit.

The rms misfit should be ~ 1 (of order unity) for a successful fit.

The residual $r(t)$ is a realization of a random process $R(t)$ with $\mathrm{E}\{R(t)\} = 0$ and $\mathrm{E}\{R^2(t)\} = \sigma^2(t)$. Here $\mathrm{E}\{\cdots\}$ denotes expectation (ensemble averaging, to be distinguished from time averaging). We normalize $D(t) = m(t) + R(t)$ by $\sigma(t)$ to obtain

$$1 = \mathrm{E}\left\{ \left(\frac{R(t)}{\sigma(t)} \right)^2 \right\} = \mathrm{E}\left\{ \left(\frac{D(t) - m(t)}{\sigma(t)} \right)^2 \right\} .$$

The normalized square misfit at time t is thus expected to be 1. The rms misfit is the square root of the time average of this expression and thus also of order unity.

Numerical Software Lab

Underfitting and overfitting

- Example: polynomial regression
- Exercise: mean square residual and model order

Least squares normal equations

- Example: polynomial fitting of synthetic data
- Example: harmonic regression of synthetic data
- Exercise: harmonic regression of QBO time series
- Exercise: SVD applied to polynomial fitting