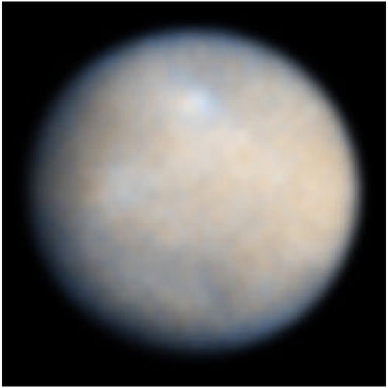
# Lecture 3 - Least Squares

- In January 1, 1801, an Italian monk Giuseppe Piazzi, discovered a faint, nomadic object through his telescope in Palermo, correctly believing it to reside in the orbital region between Mars and Jupiter.
- Piazzi watched the object for 41 days but then fell ill, and shortly thereafter the wandering star strayed into the halo of the Sun and was lost to observation.
- The newly-discovered planet had been lost, and astronomers had a mere 41 days of observation covering a tiny arc of the night from which to attempt to compute an orbit and find the planet again.

pages 1,2 are from `http://www.keplersdiscovery.com/Asteroid.html`



# Carl Friedrich Gauss

- The dean of the French astrophysical establishment, Pierre-Simon Laplace (1749-1827), declared that it simply could not be done.
- In Germany, the 24 years old German mathematician Car Friedrich Gauss had considered that this type of problem to determine a planet's orbit from a limited handful of observations - *"commended itself to mathematicians by its difficulty and elegance."*
- Gauss discovered a method for computing the planet's orbit using only three of the original observations and successfully predicted where Ceres might be found (now considered to be a dworf planet).
- The prediction catapulted him to worldwide acclaim.

# Formulation

- Consider the linear system

$$\mathbf{Ax} \approx \mathbf{b}, \quad (\mathbf{A} \in \mathbb{R}^{m \times n}, \mathbf{b} \in \mathbb{R}^m)$$

- Assumption: $\mathbf{A}$ has a full column rank, that is, $\text{rank}(\mathbf{A}) = n$.
- When $m > n$, the system is usually *inconsistent* and a common approach for finding an approximate solution is to pick the solution of the problem

$$\text{(LS)} \quad \min \|\mathbf{Ax} - \mathbf{b}\|^2.$$

# The Least Squares Solution

- The LS problem is the same as

$$\min_{\mathbf{x}\in\mathbb{R}^n} \left\{ f(\mathbf{x}) \equiv \mathbf{x}^T\mathbf{A}^T\mathbf{A}\mathbf{x} - 2\mathbf{b}^T\mathbf{A}\mathbf{x} + \|\mathbf{b}\|^2 \right\}.$$

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- $\nabla^2 f(\mathbf{x}) = 2\mathbf{A}^T\mathbf{A} \succ \mathbf{0}$
- Therefore, the unique optimal solution $\mathbf{x}_{\mathrm{LS}}$ is the solution $\nabla f(\mathbf{x}) = \mathbf{0}$, namely,

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- $\mathbf{x}_{\mathrm{LS}} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{b}$.

# A Numerical Example

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$$\begin{aligned} x_1 + 2x_2 &= 0 \\ 2x_1 + x_2 &= 1 \\ 3x_1 + 2x_2 &= 1 \end{aligned}$$

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$$\begin{pmatrix} 1 & 2 \\ 2 & 1 \\ 3 & 2 \end{pmatrix}^T \begin{pmatrix} 1 & 2 \\ 2 & 1 \\ 3 & 2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1 & 2 \\ 2 & 1 \\ 3 & 2 \end{pmatrix}^T \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix},$$

  which is the same as

$$\begin{pmatrix} 14 & 10 \\ 10 & 9 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 5 \\ 3 \end{pmatrix} \Rightarrow \mathbf{x}_{\mathrm{LS}} = \begin{pmatrix} 15/26 \\ -8/26 \end{pmatrix}.$$

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- Note that $\mathbf{A}\mathbf{x}_{\mathrm{LS}} = (-0.038; 0.846; 1.115)$, so that the errors are

$$\mathbf{b} - \mathbf{A}\mathbf{x}_{\mathrm{LS}} = \begin{pmatrix} 0.038 \\ 0.154 \\ -0.115 \end{pmatrix} \Rightarrow \text{sq. err.} = 0.038^2 + 0.154^2 + (-0.115)^2 = 0.038$$

# Data Fitting

**Linear Fitting:**

- **Data:** $(\mathbf{s}_i, t_i), i = 1, 2, \ldots, m$, where $\mathbf{s}_i \in \mathbb{R}^n$ and $t_i \in \mathbb{R}$. Assume that an approximate linear relation holds:

$$t_i \approx \mathbf{s}_i^T \mathbf{x}, \quad i = 1, 2, \ldots, m$$

- The corresponding least squares problem is:

$$\min_{\mathbf{x} \in \mathbb{R}^n} \sum_{i=1}^{m} (\mathbf{s}_i^T \mathbf{x} - t_i)^2.$$

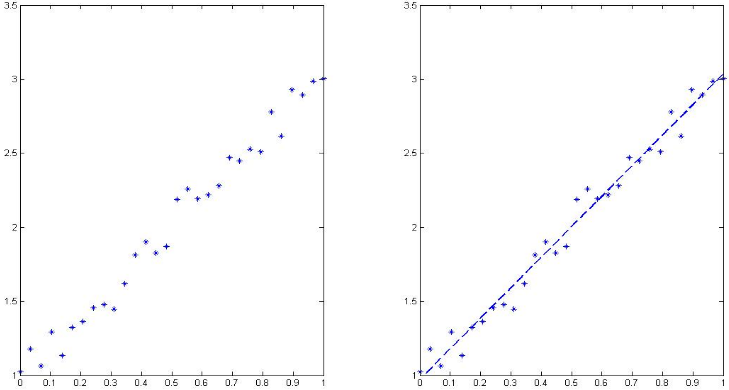
- equivalent formulation:

$$\min_{\mathbf{x} \in \mathbb{R}^n} \|\mathbf{S}\mathbf{x} - \mathbf{t}\|^2,$$

where

$$\mathbf{S} = \begin{pmatrix} - \ \mathbf{s}_1^T - \\ - \ \mathbf{s}_2^T - \\ \vdots \\ - \ \mathbf{s}_m^T - \end{pmatrix}, \mathbf{t} = \begin{pmatrix} t_1 \\ t_2 \\ \vdots \\ t_m \end{pmatrix}.$$

# Illustration



# Example of Polynomial Fitting

- Given a set of points in $\mathbb{R}^2$: $(u_i, y_i), i = 1, 2, \ldots, m$ for which the following approximate relation holds for some $a_0, \ldots, a_d$:

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- The least squares solution is of course well defined if the $m \times (d+1)$ matrix is of full column rank.
- This is true when all the $u_i$'s are different from each other (why?)

# Regularized Least Squares

- There are several situations in which the least squares solution does not give rise to a good estimate of the "true" vector $\mathbf{x}$.
- In these cases, a regularized problem (called regularized least squares (RLS)) is often solved:

$$\text{(RLS)} \quad \min_{\mathbf{x}} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2 + \lambda R(\mathbf{x}).$$

  Here $\lambda$ is the regularization parameter and $R(\cdot)$ is the regularization function (also called a penalty function).
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- The optimal solution of the above problem is

$$\mathbf{x}_{\mathrm{RLS}} = (\mathbf{A}^T\mathbf{A} + \lambda\mathbf{D}^T\mathbf{D})^{-1}\mathbf{A}^T\mathbf{b}.$$

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  what kind of assumptions are needed to assure that $\mathbf{A}^T\mathbf{A} + \lambda \mathbf{D}^T\mathbf{D}$ is invertible? (answer: $\mathrm{Null}(\mathbf{A}) \cap \mathrm{Null}(\mathbf{D}) = \{\mathbf{0}\}$)

# Application - Denoising

- Suppose that a noisy measurement of a signal $\mathbf{x} \in \mathbb{R}^n$ is given:

$$\mathbf{b} = \mathbf{x} + \mathbf{w}.$$

$\mathbf{x}$ is the unknown signal, $\mathbf{w}$ is the unknown noise and $\mathbf{b}$ is the (known) measures vector.

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  MEANINGLESS.
- Regularization is performed by exploiting some a priori information. For example, if the signal is "smooth" in some sense, then $R(\cdot)$ can be chosen as

$$R(\mathbf{x}) = \sum_{i=1}^{n-1} (x_i - x_{i+1})^2.$$

# Denoising contd.

- $R(\cdot)$ can also be written as $R(\mathbf{x}) = \|\mathbf{L}\mathbf{x}\|^2$ where $\mathbf{L} \in \mathbb{R}^{(n-1)\times n}$ is given by

$$\mathbf{L} = \begin{pmatrix} 1 & -1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 1 & -1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & -1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 & -1 \end{pmatrix}.$$

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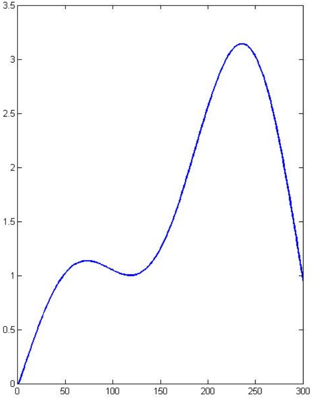
- The resulting regularized least squares problem is

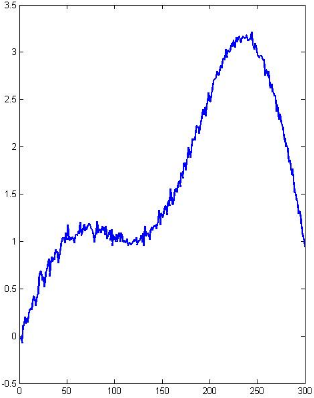
$$\min_{\mathbf{x}} \|\mathbf{x} - \mathbf{b}\|^2 + \lambda \|\mathbf{L}\mathbf{x}\|^2$$

- Hence,

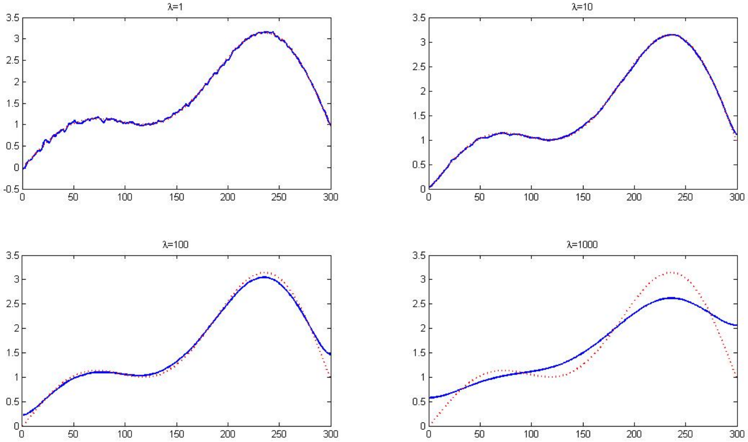
$$\mathbf{x}_{\mathrm{RLS}}(\lambda) = (\mathbf{I} + \lambda \mathbf{L}^T \mathbf{L})^{-1} \mathbf{b}.$$

# Example - true and noisy signals



# RLS reconstructions



# Nonlinear Least Squares

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- The nonlinear least squares (NLS) problem is the one of finding an $\mathbf{x}$ solving the problem

$$\min \sum_{i=1}^{m} (f_i(\mathbf{x}) - b_i)^2.$$

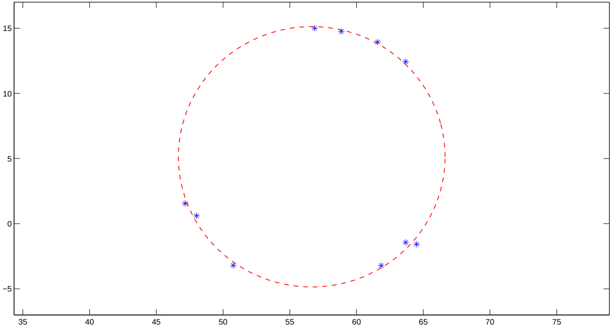
- As opposed to linear least squares, there is no easy way to to solve NLS problems. However, there are some dedicated algorithms for this problem, which we will explore later on.

# Circle Fitting – Linear Least Squares in Disguise

Given $m$ points $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_m \in \mathbb{R}^n$, the circle fitting problem seeks to find a circle

$$C(\mathbf{x}, r) = \{\mathbf{y} \in \mathbb{R}^n : \|\mathbf{y} - \mathbf{x}\| = r\}$$

that best fits the $m$ points.



# Mathematical Formulation of the CF Problem

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- Nonlinear least squares formulation:

$$\min_{\mathbf{x} \in \mathbb{R}^n, r \in \mathbb{R}_+} \sum_{i=1}^{m} (\|\mathbf{x} - \mathbf{a}_i\|^2 - r^2)^2.$$

# Reduction to a Least Squares Problem

- $$\min_{\mathbf{x},r}\left\{\sum_{i=1}^{m}(-2\mathbf{a}_i^T\mathbf{x}+\|\mathbf{x}\|^2-r^2+\|\mathbf{a}_i\|^2)^2:\mathbf{x}\in\mathbb{R}^n,r\in\mathbb{R}\right\}.$$

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- $$\min_{\mathbf{x},r} \left\{ \sum_{i=1}^m (-2\mathbf{a}_i^T\mathbf{x} + \|\mathbf{x}\|^2 - r^2 + \|\mathbf{a}_i\|^2)^2 : \mathbf{x} \in \mathbb{R}^n, r \in \mathbb{R} \right\}.$$
- Making the change of variables $R = \|\mathbf{x}\|^2 - r^2$, the above problem reduces to
$$\min_{\mathbf{x}\in\mathbb{R}^n, R\in\mathbb{R}} \left\{ f(\mathbf{x}, R) \equiv \sum_{i=1}^m (-2\mathbf{a}_i^T\mathbf{x} + R + \|\mathbf{a}_i\|^2)^2 : \|\mathbf{x}\|^2 \geq R \right\}.$$

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- The constraint $\|\mathbf{x}\|^2 \geq R$ can be dropped (will be shown soon), and therefore the problem is equivalent to the LS problem

$$\text{(CF-LS)} \ \min_{\mathbf{x},R} \left\{ \sum_{i=1}^{m} (-2\mathbf{a}_i^T\mathbf{x} + R + \|\mathbf{a}_i\|^2)^2 : \mathbf{x} \in \mathbb{R}^n, R \in \mathbb{R} \right\}.$$

# Redundancy of the Constraint $\|\mathbf{x}\|^2 \geq R$

- We will show that any optimal solution $(\hat{\mathbf{x}}, \hat{R})$ of (CF-LS) automatically satisfies $\|\hat{\mathbf{x}}\|^2 \geq \hat{R}$.

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- Otherwise, if $\|\hat{\mathbf{x}}\|^2 < \hat{R}$, then

$$-2\mathbf{a}_i^T\hat{\mathbf{x}} + \hat{R} + \|\mathbf{a}_i\|^2 > -2\mathbf{a}_i^T\hat{\mathbf{x}} + \|\hat{\mathbf{x}}\|^2 + \|\mathbf{a}_i\|^2 = \|\hat{\mathbf{x}} - \mathbf{a}_i\|^2 \geq 0, i = 1, \ldots, m.$$

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- Thus,

$$f(\hat{\mathbf{x}}, \hat{R}) = \sum_{i=1}^m \left(-2\mathbf{a}_i^T\hat{\mathbf{x}} + \hat{R} + \|\mathbf{a}_i\|^2\right)^2 > \sum_{i=1}^m \left(-2\mathbf{a}_i^T\hat{\mathbf{x}} + \|\hat{\mathbf{x}}\|^2 + \|\mathbf{a}_i\|^2\right)^2 = f(\hat{\mathbf{x}}, \|\hat{\mathbf{x}}\|^2),$$

- Contradiction to the optimality of $(\hat{\mathbf{x}}, \hat{R})$.