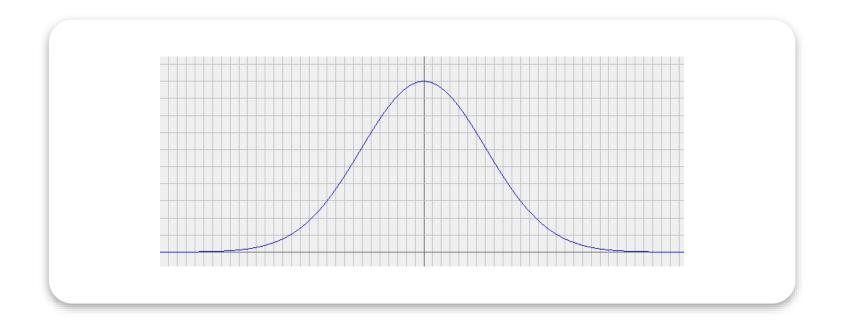
# Modelling 1 SUMMER TERM 2020







# Least-Squares

# Least-Squares Fitting

# Approximation

#### **Common Situation:**

- Many data points
  - Noisy data
  - Measurements, 3D scans, ...
- Approximate with simple curve / surface

#### What we need:

- What is a good approximation?
- How to compute?

# Approximation Techniques

# Agenda:

- Least-squares approximation (and why/when this makes sense)
- Iteratively reweighted least-squares (for nasty noise distributions)
- Total least-squares linear approximation (get rid of the coordinate system)

# Least-Squares

i.i.d. = "independent,

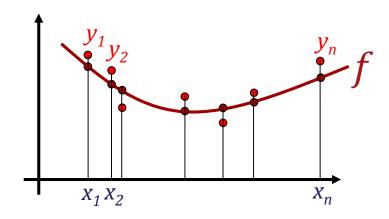
indentically

distributed"

#### Scenario for now:

- Function values  $y_i$  at positions  $x_i$  (1D  $\rightarrow$  1D)
  - Independent variables  $x_i$  known exactly.
  - Dependent variables  $y_i$  with some error.
- Error Gaussian, i.i.d.
  - normal distributed
  - independent
  - same distribution at every point
- Class of functions (basis) known

### Situation



#### Situation:

- Sample points taken at  $x_i$  from original f.
- Unknown Gaussian i.i.d. noise added to each  $y_i$ .
- Reconstruct  $\tilde{f}$ .

# Summary

Statistical model: least-squares criterion

$$\arg\min_{\tilde{f}} \sum_{i=1}^{n} (\tilde{f}(x_i) - y_i)^2$$

Linear ansatz: quadratic objective

$$\tilde{f}_{\lambda_1,\dots,\lambda_k}(x) = \sum_{j=1}^k \lambda_j b_j(x) \longrightarrow \underset{\lambda_1,\dots,\lambda_k}{\operatorname{arg min}} \sum_{i=1}^n \left( \left( \sum_{j=1}^k \lambda_j b_j(x_i) \right) - y_i \right)^{-1}$$

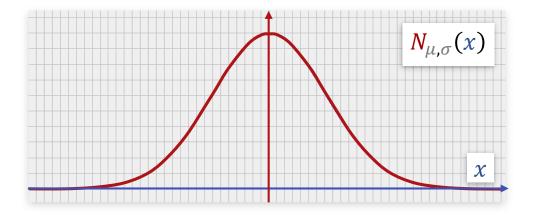
Critical point: linear system

$$\begin{pmatrix} \langle \mathbf{b}_{1}, \mathbf{b}_{1} \rangle & \cdots & \langle \mathbf{b}_{1}, \mathbf{b}_{k} \rangle \\ \vdots & \ddots & \vdots \\ \langle \mathbf{b}_{k}, \mathbf{b}_{1} \rangle & \cdots & \langle \mathbf{b}_{k}, \mathbf{b}_{k} \rangle \end{pmatrix} \begin{pmatrix} \lambda_{1} \\ \vdots \\ \lambda_{k} \end{pmatrix} = \begin{pmatrix} \langle \mathbf{y}, \mathbf{b}_{1} \rangle \\ \vdots \\ \langle \mathbf{y}, \mathbf{b}_{k} \rangle \end{pmatrix} \quad \text{with} \quad \begin{cases} \langle \mathbf{b}_{i}, \mathbf{b}_{j} \rangle \coloneqq \sum_{t=1}^{n} b_{i}(x_{t}) \cdot b_{j}(x_{t}) \\ \langle \mathbf{y}, \mathbf{b}_{i} \rangle \coloneqq \sum_{t=1}^{n} y_{t} \cdot b_{i}(x_{t})$$

#### Goal:

- Maximize probability of  $\tilde{f}$ 
  - Probability that measured data originated from  $ilde{f}$
- "Maximum likelihood estimation"

# Error Model



Gaussian normal distribution

$$N_{\mu,\sigma}(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

# **Assumption**

- Error normal distributed
  - Independent for each data point
- Gaussian noise: maximum entropy for given variance
  - Unstructured noise

$$\arg \max_{\tilde{f}} \prod_{i=1}^{n} N_{0,\sigma}(\tilde{f}(x_{i}) - y_{i}) = \arg \max_{\tilde{f}} \prod_{i=1}^{n} \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{\left(\tilde{f}(x_{i}) - y_{i}\right)^{2}}{2\sigma^{2}}\right)$$

$$= \arg \max_{\tilde{f}} \ln \left[\prod_{i=1}^{n} \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{\left(\tilde{f}(x_{i}) - y_{i}\right)^{2}}{2\sigma^{2}}\right)\right]$$

$$= \arg \max_{\tilde{f}} \sum_{i=1}^{n} \left(\left(\ln \frac{1}{\sigma\sqrt{2\pi}}\right) - \frac{\left(\tilde{f}(x_{i}) - y_{i}\right)^{2}}{2\sigma^{2}}\right)$$

$$= \arg \min_{\tilde{f}} \sum_{i=1}^{n} \left(+\frac{\left(\tilde{f}(x_{i}) - y_{i}\right)^{2}}{2\sigma^{2}}\right)$$

$$= \arg \min_{\tilde{f}} \sum_{i=1}^{n} \left(\tilde{f}(x_{i}) - y_{i}\right)^{2}$$

$$\arg\max_{\tilde{f}} \prod_{i=1}^{n} N_{0,\sigma}(\tilde{f}(x_{i}) - y_{i}) = \arg\max_{\tilde{f}} \prod_{i=1}^{n} \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{\left(\tilde{f}(x_{i}) - y_{i}\right)^{2}}{2\sigma^{2}}\right)$$

$$= \arg\max_{\tilde{f}} \ln\left[\prod_{i=1}^{n} \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{\left(\tilde{f}(x_{i}) - y_{i}\right)^{2}}{2\sigma^{2}}\right)\right]$$

$$= \arg\max_{\tilde{f}} \sum_{i=1}^{n} \left(\left(\ln\frac{1}{\sigma\sqrt{2\pi}}\right) - \frac{\left(\tilde{f}(x_{i}) - y_{i}\right)^{2}}{2\sigma^{2}}\right)$$

$$= \arg\min_{\tilde{f}} \sum_{i=1}^{n} \frac{\left(\tilde{f}(x_{i}) - y_{i}\right)^{2}}{2\sigma^{2}}$$

$$= \arg\min_{\tilde{f}} \sum_{i=1}^{n} \left(\tilde{f}(x_{i}) - y_{i}\right)^{2}$$

# Least-Squares Approximation

#### We have shown

 Maximum likelihood estimate minimizes sum of squared errors

# **Next:** Compute optimal coefficients

• Linear ansatz: 
$$\tilde{f}(x) = \sum_{j=1}^{\kappa} \lambda_j b_j(x)$$

• Determine optimal  $\lambda_i$ 

#### **Notation**

$$\lambda = \begin{pmatrix} \lambda_1 \\ \vdots \\ \lambda_k \end{pmatrix}, \quad \mathbf{b}(\mathbf{x}) = \begin{pmatrix} b_1(\mathbf{x}) \\ \vdots \\ b_k(\mathbf{x}) \end{pmatrix}, \quad \mathbf{b}_i = \begin{pmatrix} b_i(x_1) \\ \vdots \\ b_i(x_n) \end{pmatrix}, \quad \mathbf{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$$

$$\uparrow k \text{ entries} \qquad \uparrow n \text{ entries} \qquad \uparrow n \text{ entries}$$

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$$\uparrow k \text{ entries} \qquad \uparrow k \text{ entries} \qquad \uparrow n \text{ entries}$$

$$\arg\min_{\tilde{f}} \sum_{i=1}^{n} (\tilde{f}(x_i) - y_i)^2 = \arg\min_{\lambda} \sum_{i=1}^{n} \left( \sum_{j=1}^{k} \lambda_j b_j(x_i) - y_i \right)^2$$

$$= \arg\min_{\lambda} \sum_{i=1}^{n} (\lambda^T \mathbf{b}(x_i) - y_i)^2$$

$$= \arg\min_{\lambda} \lambda^T \left[ \sum_{i=1}^{n} \mathbf{b}(x_i) \mathbf{b}^T(x_i) \right] \lambda - 2 \sum_{i=1}^{n} y_i \lambda^T \mathbf{b}(x_i) + \sum_{i=1}^{n} y_i^2$$

$$\lambda = \begin{pmatrix} \lambda_1 \\ \vdots \\ \lambda_k \end{pmatrix}, \quad \mathbf{b}(\mathbf{x}) = \begin{pmatrix} b_1(\mathbf{x}) \\ \vdots \\ b_k(\mathbf{x}) \end{pmatrix}, \quad \mathbf{b}_i = \begin{pmatrix} b_i(x_1) \\ \vdots \\ b_i(x_n) \end{pmatrix}, \quad \mathbf{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$$

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$$\mathbf{x}^T \mathbf{A} \mathbf{x} \qquad \mathbf{b} \mathbf{x} \qquad C$$

→ quadratic optimization problem

### Critical Point

$$\lambda = \begin{pmatrix} \lambda_1 \\ \vdots \\ \lambda_k \end{pmatrix}, \quad \mathbf{b}(\mathbf{x}) = \begin{pmatrix} b_1(\mathbf{x}) \\ \vdots \\ b_k(\mathbf{x}) \end{pmatrix}, \quad \mathbf{b}_i = \begin{pmatrix} b_i(x_1) \\ \vdots \\ b_i(x_n) \end{pmatrix}, \quad \mathbf{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$$

$$\uparrow k \text{ entries} \qquad \uparrow k \text{ entries} \qquad \uparrow n \text{ entries}$$

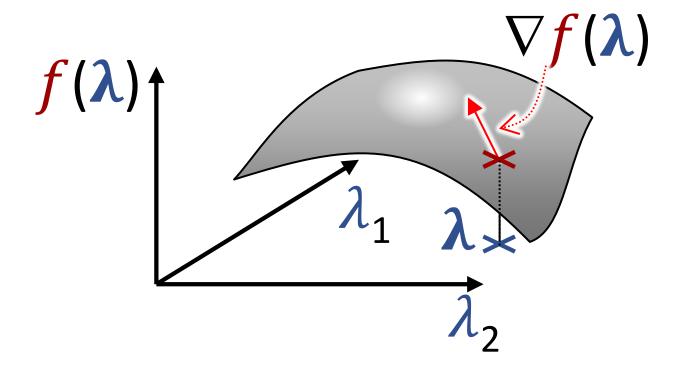
$$\nabla_{\lambda} \left( \lambda^{T} \left[ \sum_{i=1}^{n} \mathbf{b}(x_{i}) \mathbf{b}^{T}(x_{i}) \right] \lambda - 2 \sum_{i=1}^{n} y_{i} \lambda^{T} \mathbf{b}(x_{i}) + \sum_{i=1}^{n} y_{i}^{2} \right) \leftarrow \text{Find minimum (critical point)}$$

$$= 2\left[\sum_{i=1}^{n} \mathbf{b}(x_i) \mathbf{b}^{\mathrm{T}}(x_i)\right] \lambda - 2\sum_{i=1}^{n} y_i \mathbf{b}(x_i)$$

### **Linear System:**

$$\left[\sum_{i=1}^{n} \mathbf{b}(x_i) \mathbf{b}^{\mathrm{T}}(x_i)\right] \boldsymbol{\lambda} = \begin{pmatrix} \mathbf{y}^{\mathrm{T}} \mathbf{b}_1 \\ \vdots \\ \mathbf{y}^{\mathrm{T}} \mathbf{b}_k \end{pmatrix}$$

# Gradient



#### Critical Point

$$\lambda = \begin{pmatrix} \lambda_1 \\ \vdots \\ \lambda_k \end{pmatrix}, \quad \mathbf{b}(\mathbf{x}) = \begin{pmatrix} b_1(\mathbf{x}) \\ \vdots \\ b_k(\mathbf{x}) \end{pmatrix}, \quad \mathbf{b}_i = \begin{pmatrix} b_i(x_1) \\ \vdots \\ b_i(x_n) \end{pmatrix}, \quad \mathbf{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$$

$$\uparrow k \text{ entries} \qquad \uparrow n \text{ entries} \qquad \uparrow n \text{ entries}$$

#### **Linear System**

$$\left[\sum_{i=1}^{n} \mathbf{b}(x_i) \mathbf{b}^{\mathrm{T}}(x_i)\right] \boldsymbol{\lambda} = \begin{pmatrix} \mathbf{y}^{\mathrm{T}} \mathbf{b}_1 \\ \vdots \\ \mathbf{y}^{\mathrm{T}} \mathbf{b}_k \end{pmatrix}$$

#### Can be written as

$$\begin{pmatrix} \langle \mathbf{b}_{1}, \mathbf{b}_{1} \rangle & \cdots & \langle \mathbf{b}_{1}, \mathbf{b}_{k} \rangle \\ \vdots & \ddots & \vdots \\ \langle \mathbf{b}_{k}, \mathbf{b}_{1} \rangle & \cdots & \langle \mathbf{b}_{k}, \mathbf{b}_{k} \rangle \end{pmatrix} \begin{pmatrix} \lambda_{1} \\ \vdots \\ \lambda_{k} \end{pmatrix} = \begin{pmatrix} \langle \mathbf{y}, \mathbf{b}_{1} \rangle \\ \vdots \\ \langle \mathbf{y}, \mathbf{b}_{k} \rangle \end{pmatrix} \text{ with } \begin{cases} \langle \mathbf{b}_{i}, \mathbf{b}_{j} \rangle \coloneqq \sum_{t=1}^{n} b_{i}(x_{t}) \cdot b_{j}(x_{t}) \\ \langle \mathbf{y}, \mathbf{b}_{i} \rangle \coloneqq \sum_{t=1}^{n} y_{t} \cdot b_{i}(x_{t}) \end{cases}$$

# Summary (again)

Statistical model: least-squares criterion

$$\arg\min_{\tilde{f}} \sum_{i=1}^{n} (\tilde{f}(x_i) - y_i)^2$$

Linear ansatz: quadratic objective

$$\tilde{f}_{\lambda_1,\dots,\lambda_k}(x) = \sum_{j=1}^k \lambda_j b_j(x) \quad \Longrightarrow \quad \underset{\lambda_1,\dots,\lambda_k}{\operatorname{arg \, min}} \sum_{i=1}^n \left( \left( \sum_{j=1}^k \lambda_j b_j(x_i) \right) - y_i \right)^2$$

Critical point: linear system

### Variants

### Weighted least squares:

- Varying noise level
  - Varying standard deviations  $\sigma_i$
- Weighted least squares problem
- Noisier points have smaller influence

# Same procedure as prev. slides...

$$\arg\max_{\tilde{f}} \prod_{i=1}^{n} N_{0,\sigma_{i}}(\tilde{f}(x_{i}) - y_{i}) = \arg\max_{\tilde{f}} \prod_{i=1}^{n} \frac{1}{\sigma_{i}\sqrt{2\pi}} \exp\left(-\frac{\left(\tilde{f}(x_{i}) - y_{i}\right)^{2}}{2\sigma_{i}^{2}}\right)$$

$$= \arg\max_{\tilde{f}} \ln\left[\prod_{i=1}^{n} \frac{1}{\sigma_{i}\sqrt{2\pi}} \exp\left(-\frac{\left(\tilde{f}(x_{i}) - y_{i}\right)^{2}}{2\sigma_{i}^{2}}\right)\right]$$

$$= \arg\max_{\tilde{f}} \sum_{i=1}^{n} \left(\left(\ln\frac{1}{\sigma_{i}\sqrt{2\pi}}\right) - \frac{\left(\tilde{f}(x_{i}) - y_{i}\right)^{2}}{2\sigma_{i}^{2}}\right)$$

$$= \arg\min_{\tilde{f}} \sum_{i=1}^{n} \frac{\left(\tilde{f}(x_{i}) - y_{i}\right)^{2}}{2\sigma_{i}^{2}}$$

$$= \arg\min_{\tilde{f}} \sum_{i=1}^{n} \frac{1}{\sigma_{i}^{2}} \left(\tilde{f}(x_{i}) - y_{i}\right)^{2}$$

### Result

#### Linear system for the general case:

$$\begin{pmatrix} \langle \mathbf{b}_{1}, \mathbf{b}_{1} \rangle & \cdots & \langle \mathbf{b}_{1}, \mathbf{b}_{k} \rangle \\ \vdots & \ddots & \vdots \\ \langle \mathbf{b}_{k}, \mathbf{b}_{1} \rangle & \cdots & \langle \mathbf{b}_{k}, \mathbf{b}_{k} \rangle \end{pmatrix} \begin{pmatrix} \lambda_{1} \\ \vdots \\ \lambda_{k} \end{pmatrix} = \begin{pmatrix} \langle \mathbf{y}, \mathbf{b}_{1} \rangle \\ \vdots \\ \langle \mathbf{y}, \mathbf{b}_{k} \rangle \end{pmatrix} \text{ with } \begin{cases} \langle \mathbf{b}_{i}, \mathbf{b}_{j} \rangle \coloneqq \sum_{t=1}^{n} b_{i}(x_{t}) \cdot b_{j}(x_{t}) \cdot \frac{\omega^{2}(x_{t})}{\omega^{2}(x_{t})} \\ \langle \mathbf{y}, \mathbf{b}_{i} \rangle \coloneqq \sum_{t=1}^{n} y_{t} \cdot b_{i}(x_{t}) \cdot \omega^{2}(x_{t}) \end{cases}$$

$$\omega^2(x_t) = \frac{1}{\sigma_t^2}$$
, i.e.  $\omega(x_t) = \frac{1}{\sigma_t}$ 

# Larger $\omega \rightarrow$ larger influence of data point

# Least-Squares Linear Systems

# Least-squares solution to general linear system

Consider

$$Ax = b$$

Least-squares formulation

$$\arg \min_{\mathbf{x} \in \mathbb{R}^d} (\mathbf{A}\mathbf{x} - \mathbf{b})^2$$

$$= \arg \min_{\mathbf{x} \in \mathbb{R}^d} (\mathbf{x}^T \mathbf{A}^T \mathbf{A}\mathbf{x} - 2\mathbf{b}^T \mathbf{A}\mathbf{x} + \mathbf{b}^T \mathbf{b})$$

$$\mathbf{x} \in \mathbb{R}^d$$

Critical point: gradient = zero

$$\mathbf{A}^{\mathrm{T}}\mathbf{A}\mathbf{x} = \mathbf{A}^{\mathrm{T}}\mathbf{b}$$

"System of normal equations"

### SVD

### Problem with normal equations:

- Condition number for normal equations
   = (condition number of A)<sup>2</sup>
- Proof
  - SVD:  $\mathbf{A} = \mathbf{U} \mathbf{D} \mathbf{V}^{\mathrm{T}}$
  - $\bullet \mathbf{A}^{\mathrm{T}}\mathbf{A} = \mathbf{V} \mathbf{D} \mathbf{U}^{\mathrm{T}} \mathbf{U} \mathbf{D} \mathbf{V}^{\mathrm{T}} = \mathbf{V}^{\mathrm{T}}\mathbf{D}^{2}\mathbf{V}$
- More stable (for bad problems)
  - Use SVD:
  - $A^{-1} \approx A^{+} = V D^{+} U^{T}$ ("+" = pseudo-inverse, do not invert zero singular values)
- Effect: Pick smallest solution to normal Equations

# Connection to Least-Squares Approx.

### **Equivalent results:**

 Least-squares fitting of basis functions to data same as

- Setting up over-constrained interpolation problem
- Then solve system of normal equations
  - Or pseudoinverse

#### **Proof**

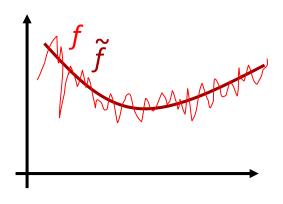
Elementary: Compare resulting equations

# One more Variant...

# **Function Approximation**

- Function given
  - $f: \Omega \supseteq \mathbb{R}^n \to \mathbb{R}$
  - Approximate by

$$\widetilde{f_{\lambda}} = \sum_{i=1}^{d} \lambda_i b_i$$



- Difference: Continuous function as "data"
- Almost the same solution...

# **Function Approximation**

### **Objective function:**

- $\|\tilde{f}(\mathbf{x}) f\|^2 \to \min$
- Solution

$$\left\| \sum_{i=1}^{k} \lambda_{i} b_{i} - f \right\|^{2} = \left( \sum_{i=1}^{k} \lambda_{i} b_{i} - f, \sum_{i=1}^{k} \lambda_{i} b_{i} - f \right)$$

$$= \lambda^{T} \begin{pmatrix} \langle b_{1}, b_{1} \rangle & \cdots & \langle b_{k}, b_{1} \rangle \\ \vdots & & \vdots \\ \langle b_{1}, b_{k} \rangle & \cdots & \langle b_{k}, b_{k} \rangle \end{pmatrix} \lambda - \sum_{i=1}^{k} \lambda_{i} \langle b_{i}, f \rangle + \langle f, f \rangle$$

# **Function Approximation**

# Critical point (i.e., solution):

$$\begin{pmatrix} \langle b_1, b_1 \rangle & \cdots & \langle b_k, b_1 \rangle \\ \vdots & & \vdots \\ \langle b_1, b_k \rangle & \cdots & \langle b_k, b_k \rangle \end{pmatrix} \begin{pmatrix} \lambda_1 \\ \vdots \\ \lambda_k \end{pmatrix} = \begin{pmatrix} \langle f, b_1 \rangle \\ \vdots \\ \langle f, b_k \rangle \end{pmatrix}$$

#### with:

$$\langle f, g \rangle = \int_{\Omega} f(\mathbf{x}) g(\mathbf{x}) d\mathbf{x}, (\Omega \subseteq \mathbb{R}^D)$$
 (unweighted version)

or

$$\langle f, g \rangle = \int_{\Omega} f(\mathbf{x}) g(\mathbf{x}) \omega^2(\mathbf{x}) d\mathbf{x}, (\Omega \subseteq \mathbb{R}^D)$$
 (weighted version)

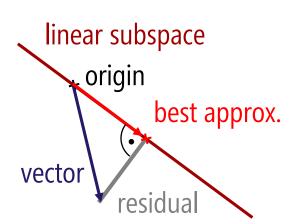
# Galerkin Approximation

### Least-squares criterion (here) equivalent to:

residual each basis function 
$$\forall i \in \{1, ..., k\}: \left(\sum_{j=1}^{k} \lambda_j b_j - f, b_i\right) = 0$$

$$\Leftrightarrow \forall i \in \{1, \dots, k\} : \left(\sum_{j=1}^{k} \lambda_{j} b_{j}, b_{i}\right) = \langle f, b_{i} \rangle$$

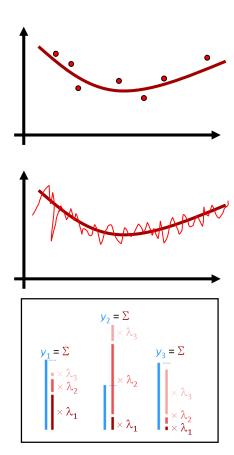
$$\Leftrightarrow \begin{pmatrix} \langle b_1, b_1 \rangle & \cdots & \langle b_k, b_1 \rangle \\ \vdots & & \vdots \\ \langle b_1, b_k \rangle & \cdots & \langle b_k, b_k \rangle \end{pmatrix} \begin{pmatrix} \lambda_1 \\ \vdots \\ \lambda_k \end{pmatrix} = \begin{pmatrix} \langle f, b_1 \rangle \\ \vdots \\ \langle f, b_k \rangle \end{pmatrix}$$



# Summary

#### What we can do so far:

- Least-squares approximation:
  - Fit linear combination to data points
- Variants
  - Solve linear systems approximately
  - Fit functions to functions
- Extensions
  - Weights model varying uncertainty
  - The multi-dimensional case is similar



# Remaining problems

# What is missing:

- Gaussian noise only
  - → Iteratively reweighted least-squares (M-estimators)
- Errors in x-direction are ignored
  - → Total least-squares