

CS189: Intro to Machine Learning

Summer 2018

Lecture 6: Maximum Likelihood and Maximum a Posteriori, pt. 2

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Goal for today

Generic MAP regression

- multivariate gaussian observation noise
- multivariate gaussian prior on parameters

Approach we'll take

Generalize our current MAP estimate a bit at a time

- *Weighted least squares:* Remove the “identically distributed” assumption from the output noise z (where $y = f(x) + z$)
- *Generalized least squares:* Remove the “independent” assumption from z
- *MAP with colored noise:* Remove i.i.d assumptions from parameter prior

Outline

- Weighted least squares
- Generalized least squares
- MAP with colored noise

Outline

- **Weighted least squares**
- Generalized least squares
- MAP with colored noise

Revisiting the iid assumptions

OLS assumptions

$$y_i = f(\vec{x}_i) + z_i \qquad z_i \stackrel{\text{iid}}{\sim} \mathcal{N}(0, \sigma^2)$$



Equivalent to the following:

$$\vec{z} \sim \mathcal{N}(\vec{0}, \sigma^2 I)$$

Revisiting the iid assumptions

OLS assumptions

$$y_i = f(\vec{x}_i) + z_i \qquad \vec{z} \sim \mathcal{N}(\vec{0}, \sigma^2 I)$$

WLS assumptions

$$y_i = f(\vec{x}_i) + z_i \qquad \vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z)$$

$\downarrow$
i.e.,
 $z_i \sim \mathcal{N}(0, \sigma_i^2)$

$$\Sigma_z = \begin{bmatrix} \sigma_1^2 & 0 & \cdots & 0 \\ 0 & \sigma_2^2 & \cdots & 0 \\ \vdots & & & \vdots \\ 0 & 0 & \cdots & \sigma_n^2 \end{bmatrix}$$

Revisiting the iid assumptions

OLS assumptions

$$y_i = f(\vec{x}_i) + z_i \qquad \vec{z} \sim \mathcal{N}(\vec{0}, \sigma^2 I)$$

WLS assumptions

$$y_i = f(\vec{x}_i) + z_i \qquad \vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z)$$

$\downarrow$
i.e.,

Independent, but not identically distributed $\longrightarrow z_i \sim \mathcal{N}(0, \sigma_i^2)$

$$\Sigma_z = \begin{bmatrix} \sigma_1^2 & 0 & \dots & 0 \\ 0 & \sigma_2^2 & \dots & 0 \\ \vdots & & & \vdots \\ 0 & 0 & \dots & \sigma_n^2 \end{bmatrix}$$

Deriving the WLS optimization problem

WLS assumptions

$$y_i = f(\vec{x}_i) + z_i \quad \vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z) \quad \Sigma_z = \begin{bmatrix} \sigma_1^2 & \cdots & 0 \\ \vdots & & \vdots \\ 0 & \cdots & \sigma_n^2 \end{bmatrix}$$

Key idea

Find a transformation that turns this problem into OLS.

The *reparameterization trick*.

Deriving the WLS optimization problem

WLS assumptions

$$y_i = f(\vec{x}_i) + z_i \quad \vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z) \quad \Sigma_z = \begin{bmatrix} \sigma_1^2 & \cdots & 0 \\ \vdots & & \vdots \\ 0 & \cdots & \sigma_n^2 \end{bmatrix}$$

Derivation of WLS

Perform the following transformation

$$\frac{y_i}{\sigma_i} = \frac{f(\vec{x}_i)}{\sigma_i} + \frac{z_i}{\sigma_i}$$

Deriving the WLS optimization problem

WLS assumptions

$$y_i = f(\vec{x}_i) + z_i \quad \vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z) \quad \Sigma_z = \begin{bmatrix} \sigma_1^2 & \cdots & 0 \\ \vdots & & \vdots \\ 0 & \cdots & \sigma_n^2 \end{bmatrix}$$

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Deriving the WLS optimization problem

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Derivation of WLS

Perform the following transformation

$$\frac{y_i}{\sigma_i} = \frac{f(\vec{x}_i)}{\sigma_i} + \frac{z_i}{\sigma_i}$$
$$\frac{z_i}{\sigma_i} \stackrel{iid}{\sim}$$

Deriving the WLS optimization problem

WLS assumptions

$$y_i = f(\vec{x}_i) + z_i \quad \vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z) \quad \Sigma_z = \begin{bmatrix} \sigma_1^2 & \cdots & 0 \\ \vdots & & \vdots \\ 0 & \cdots & \sigma_n^2 \end{bmatrix}$$

Derivation of WLS

Perform the following transformation

$$\frac{y_i}{\sigma_i} = \frac{f(\vec{x}_i)}{\sigma_i} + \frac{z_i}{\sigma_i}$$

$$\frac{z_i}{\sigma_i} \stackrel{iid}{\sim} \mathcal{N}(0, 1)$$

Deriving the WLS optimization problem

WLS assumptions

$$y_i = f(\vec{x}_i) + z_i \quad \vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z) \quad \Sigma_z = \begin{bmatrix} \sigma_1^2 & \cdots & 0 \\ \vdots & & \vdots \\ 0 & \cdots & \sigma_n^2 \end{bmatrix}$$

Derivation of WLS

Write the change of coordinates as follows:

Deriving the WLS optimization problem

WLS assumptions

$$y_i = f(\vec{x}_i) + z_i \quad \vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z) \quad \Sigma_z = \begin{bmatrix} \sigma_1^2 & \cdots & 0 \\ \vdots & & \vdots \\ 0 & \cdots & \sigma_n^2 \end{bmatrix}$$

Derivation of WLS

Write the change of coordinates as follows:

$$\Sigma_z^{-\frac{1}{2}} y$$

Deriving the WLS optimization problem

WLS assumptions

$$y_i = f(\vec{x}_i) + z_i \quad \vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z) \quad \Sigma_z = \begin{bmatrix} \sigma_1^2 & \cdots & 0 \\ \vdots & & \vdots \\ 0 & \cdots & \sigma_n^2 \end{bmatrix}$$

Derivation of WLS

Write the change of coordinates as follows:

$$\Sigma_z^{-\frac{1}{2}} y \sim$$

Deriving the WLS optimization problem

WLS assumptions

$$y_i = f(\vec{x}_i) + z_i \quad \vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z) \quad \Sigma_z = \begin{bmatrix} \sigma_1^2 & \cdots & 0 \\ \vdots & & \vdots \\ 0 & \cdots & \sigma_n^2 \end{bmatrix}$$

Derivation of WLS

Write the change of coordinates as follows:

$$\Sigma_z^{-\frac{1}{2}} y \sim \mathcal{N}(\vec{0}, \Sigma_z^{-\frac{1}{2}})$$

Deriving the WLS optimization problem

WLS assumptions

$$y_i = f(\vec{x}_i) + z_i \quad \vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z) \quad \Sigma_z = \begin{bmatrix} \sigma_1^2 & \cdots & 0 \\ \vdots & & \vdots \\ 0 & \cdots & \sigma_n^2 \end{bmatrix}$$

Derivation of WLS

Write the change of coordinates as follows:

$$\Sigma_z^{-\frac{1}{2}} y \sim \mathcal{N}(\Sigma_z^{-\frac{1}{2}} X w$$

Deriving the WLS optimization problem

WLS assumptions

$$y_i = f(\vec{x}_i) + z_i \quad \vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z) \quad \Sigma_z = \begin{bmatrix} \sigma_1^2 & \cdots & 0 \\ \vdots & & \vdots \\ 0 & \cdots & \sigma_n^2 \end{bmatrix}$$

Derivation of WLS

Write the change of coordinates as follows:

$$\Sigma_z^{-\frac{1}{2}} y \sim \mathcal{N}(\Sigma_z^{-\frac{1}{2}} X w, I)$$

Deriving the WLS optimization problem

WLS assumptions

$$y_i = f(\vec{x}_i) + z_i \quad \vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z) \quad \Sigma_z = \begin{bmatrix} \sigma_1^2 & \cdots & 0 \\ \vdots & & \vdots \\ 0 & \cdots & \sigma_n^2 \end{bmatrix}$$
$$\Sigma_z^{-\frac{1}{2}} y \sim \mathcal{N}(\Sigma_z^{-\frac{1}{2}} X w, I)$$

Derivation of WLS

$$\hat{w}_{WLS}$$

Deriving the WLS optimization problem

WLS assumptions

$$y_i = f(\vec{x}_i) + z_i \quad \vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z)$$
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Derivation of WLS

$$\hat{w}_{WLS} = \arg \min_w$$

Deriving the WLS optimization problem

WLS assumptions

$$y_i = f(\vec{x}_i) + z_i \quad \vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z)$$
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Derivation of WLS

$$\hat{w}_{WLS} = \arg \min_w \left(\sum_{i=1}^n \frac{\left(\frac{y_i}{\sigma_i} - \frac{\vec{x}_i^T}{\sigma_i} w \right)^2}{2} \right)$$

Deriving the WLS optimization problem

WLS assumptions

$$y_i = f(\vec{x}_i) + z_i \quad \vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z)$$
$$\Sigma_z = \begin{bmatrix} \sigma_1^2 & \cdots & 0 \\ \vdots & & \vdots \\ 0 & \cdots & \sigma_n^2 \end{bmatrix}$$
$$\Sigma_z^{-\frac{1}{2}} y \sim \mathcal{N}(\Sigma_z^{-\frac{1}{2}} X w, I)$$

Derivation of WLS

$$\hat{w}_{WLS} = \arg \min_w \left(\sum_{i=1}^n \frac{\left(\frac{y_i}{\sigma_i} - \frac{\vec{x}_i^T}{\sigma_i} w \right)^2}{2} \right) + n \log \sqrt{2\pi}$$

Deriving the WLS optimization problem

WLS assumptions

$$y_i = f(\vec{x}_i) + z_i \quad \vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z)$$
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$$= \arg \min_w$$

Deriving the WLS optimization problem

WLS assumptions

$$y_i = f(\vec{x}_i) + z_i \quad \vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z)$$
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Derivation of WLS

$$\hat{w}_{WLS} = \arg \min_w \left(\sum_{i=1}^n \frac{\left(\frac{y_i}{\sigma_i} - \frac{\vec{x}_i^T}{\sigma_i} w \right)^2}{2} \right) + n \log \sqrt{2\pi}$$
$$= \arg \min_w \sum_{i=1}^n \frac{1}{\sigma_i^2}$$

Deriving the WLS optimization problem

WLS assumptions

$$y_i = f(\vec{x}_i) + z_i \quad \vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z)$$
$$\Sigma_z = \begin{bmatrix} \sigma_1^2 & \cdots & 0 \\ \vdots & & \vdots \\ 0 & \cdots & \sigma_n^2 \end{bmatrix}$$
$$\Sigma_z^{-\frac{1}{2}} y \sim \mathcal{N}(\Sigma_z^{-\frac{1}{2}} X w, I)$$

Derivation of WLS

$$\hat{w}_{WLS} = \arg \min_w \left(\sum_{i=1}^n \frac{\left(\frac{y_i}{\sigma_i} - \frac{\vec{x}_i^T}{\sigma_i} w \right)^2}{2} \right) + n \log \sqrt{2\pi}$$
$$= \arg \min_w \sum_{i=1}^n \frac{1}{\sigma_i^2} (y_i - \vec{x}_i^T w)^2$$

WLS intuition

$$\hat{w}_{WLS} = \arg \min_w \sum_{i=1}^n \frac{1}{\sigma_i^2} (y_i - \vec{x}_i^T w)^2$$

- Same as OLS, except the loss for each data point is scaled by some factor
- Probabilistically, this factor is the inverse of the variance
- Data points assumed to have more noise should be given less weight

WLS optimization problem

$$\begin{aligned}\hat{w}_{WLS} &= \arg \min_w \sum_{i=1}^n \frac{1}{\sigma_i^2} (y_i - \vec{x}_i^T w)^2 \\ &= \arg \min_w (y - Xw)^T \Omega (y - Xw) \quad \left[\Omega = \text{diag} \left(\frac{1}{\sigma_1^2}, \dots, \frac{1}{\sigma_n^2} \right) \right] \\ &= \arg \min_w (y - Xw)^T \Omega^{1/2} \Omega^{1/2} (y - Xw) \\ &= \arg \min_w (\Omega^{1/2} y - \Omega^{1/2} Xw)^T (\Omega^{1/2} y - \Omega^{1/2} Xw) \\ &= \left((\Omega^{1/2} X)^T (\Omega^{1/2} X) \right)^{-1} \left(\Omega^{1/2} X \right)^T \Omega^{1/2} y \\ &= (X^T \Omega X)^{-1} X^T \Omega y\end{aligned}$$

WLS summary

Probabilistic assumptions

$$y_i = f(\vec{x}_i) + z_i \quad \vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z) \quad \Sigma_z = \begin{bmatrix} \sigma_1^2 & \cdots & 0 \\ \vdots & & \vdots \\ 0 & \cdots & \sigma_n^2 \end{bmatrix}$$

Optimization problem

$$\hat{w}_{WLS} = \arg \min_w \sum_{i=1}^n \frac{1}{\sigma_i^2} (y_i - \vec{x}_i^T w)^2 = \arg \min_w (y - Xw)^T \Omega (y - Xw)$$

Solution

$$\hat{w}_{WLS} = (X^T \Omega X)^{-1} X^T \Omega y$$

Outline

- Weighted least squares
- **Generalized least squares**
- MAP with colored noise

Revisiting the iid assumptions

OLS assumptions

$$y_i = f(\vec{x}_i) + z_i \qquad \vec{z} \sim \mathcal{N}(\vec{0}, \sigma^2 I)$$

WLS assumptions

$$y_i = f(\vec{x}_i) + z_i \qquad \vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z)$$

$\downarrow$
i.e.,
 $z_i \sim \mathcal{N}(0, \sigma_i^2)$

$$\Sigma_z = \begin{bmatrix} \sigma_1^2 & 0 & \cdots & 0 \\ 0 & \sigma_2^2 & \cdots & 0 \\ \vdots & & & \vdots \\ 0 & 0 & \cdots & \sigma_n^2 \end{bmatrix}$$

Revisiting the iid assumptions

OLS assumptions

$$y_i = f(\vec{x}_i) + z_i \qquad \vec{z} \sim \mathcal{N}(\vec{0}, \sigma^2 I)$$

GLS assumptions

$$y_i = f(\vec{x}_i) + z_i \qquad \vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z) \qquad \Sigma_z = \text{Any covariance matrix}$$

↑
Neither independent nor
identically distributed!

Deriving the GLS optimization problem

GLS assumptions

$$y_i = f(\vec{x}_i) + z_i$$

$$\vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z)$$

$\Sigma_z =$ Any covariance matrix

Key idea

Find a transformation that turns this problem into OLS.

The *reparameterization trick*.

Deriving the GLS optimization problem

GLS assumptions

$$y_i = f(\vec{x}_i) + z_i$$

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Derivation of GLS

$$\hat{w}_{\text{GLS}}$$

Deriving the GLS optimization problem

GLS assumptions

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Derivation of GLS

$$\hat{w}_{\text{GLS}} = \arg \max_w$$

Deriving the GLS optimization problem

GLS assumptions

$$y_i = f(\vec{x}_i) + z_i$$

$$\vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z)$$

$\Sigma_z =$ Any covariance matrix

Derivation of GLS

$$\hat{w}_{\text{GLS}} = \arg \max_w \frac{1}{\sqrt{\det(\Sigma_z)}}$$

Deriving the GLS optimization problem

GLS assumptions

$$y_i = f(\vec{x}_i) + z_i$$

$$\vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z)$$

$\Sigma_z =$ Any covariance matrix

Derivation of GLS

$$\hat{w}_{\text{GLS}} = \arg \max_w \frac{1}{\sqrt{\det(\Sigma_z)}} \frac{1}{\sqrt{(2\pi)^n}}$$

Deriving the GLS optimization problem

GLS assumptions

$$y_i = f(\vec{x}_i) + z_i$$

$$\vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z)$$

$\Sigma_z =$ Any covariance matrix

Derivation of GLS

$$\hat{w}_{\text{GLS}} = \arg \max_w \frac{1}{\sqrt{\det(\Sigma_z)}} \frac{1}{\sqrt{(2\pi)^n}} \exp \left(-\frac{1}{2} (Y - Xw)^T \Sigma_z^{-1} (Y - Xw) \right)$$

Deriving the GLS optimization problem

GLS assumptions

$$y_i = f(\vec{x}_i) + z_i$$

$$\vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z)$$

$\Sigma_z =$ Any covariance matrix

Derivation of GLS

$$\hat{w}_{\text{GLS}} = \arg \max_w \frac{1}{\sqrt{\det(\Sigma_z)}} \frac{1}{\sqrt{(2\pi)^n}} \exp \left(-\frac{1}{2} (Y - Xw)^T \Sigma_z^{-1} (y - Xw) \right)$$

$$= \arg \min_w$$

Deriving the GLS optimization problem

GLS assumptions

$$y_i = f(\vec{x}_i) + z_i$$

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Derivation of GLS

$$\hat{w}_{\text{GLS}} = \arg \max_w \frac{1}{\sqrt{\det(\Sigma_z)}} \frac{1}{\sqrt{(2\pi)^n}} \exp \left(-\frac{1}{2} (Y - Xw)^T \Sigma_z^{-1} (y - Xw) \right)$$

$$= \arg \min_w (y - Xw)^T \Sigma_z^{-1} (y - Xw)$$

Deriving the GLS optimization problem

GLS assumptions

$$y_i = f(\vec{x}_i) + z_i$$

$$\vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z)$$

$\Sigma_z =$ Any covariance matrix

Derivation of GLS

$$\hat{w}_{\text{GLS}} = \arg \min_w (y - Xw)^T \Sigma_z^{-1} (y - Xw)$$

Spectral decomposition of Sigma

$$\Sigma_z = Q \operatorname{diag}(\sigma_1^2, \dots, \sigma_n^2) Q^T$$

$$\Sigma_z^{-\frac{1}{2}} = Q \operatorname{diag}\left(\frac{1}{\sigma_1}, \dots, \frac{1}{\sigma_n}\right) Q^T$$

Deriving the GLS optimization problem

GLS assumptions

$$y_i = f(\vec{x}_i) + z_i$$

$$\vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z)$$

$\Sigma_z =$ Any covariance matrix

Derivation of GLS

$$\begin{aligned}\hat{w}_{\text{GLS}} &= \arg \min_w (y - Xw)^T \Sigma_z^{-1} (y - Xw) \\ &= \arg \min_w (y - Xw)^T \Sigma^{-\frac{1}{2}} \Sigma^{-\frac{1}{2}} (y - Xw) \\ &= \arg \min_w (\Sigma^{-\frac{1}{2}} y - \Sigma^{-\frac{1}{2}} Xw)^T (\Sigma^{-\frac{1}{2}} y - \Sigma^{-\frac{1}{2}} Xw) \\ &= \left((\Sigma^{-\frac{1}{2}} X)^T (\Sigma^{-\frac{1}{2}} X) \right)^{-1} (\Sigma^{-\frac{1}{2}} X)^T \Sigma^{-\frac{1}{2}} y \\ &= (X^T \Sigma_z^{-1} X)^{-1} X^T \Sigma_z^{-1} y\end{aligned}$$

GLS summary

Probabilistic assumptions

$$y_i = f(\vec{x}_i) + z_i \qquad \vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z) \qquad \Sigma_z = \text{Any covariance matrix}$$

Optimization problem

$$\hat{w}_{\text{GLS}} = \arg \min_w (y - Xw)^T \Sigma_z^{-1} (y - Xw)$$

Solution

$$\hat{w}_{\text{GLS}} = \left(X^T \Sigma_z^{-1} X \right)^{-1} X^T \Sigma_z^{-1} y$$

Outline

- Weighted least squares
- Generalized least squares
- **MAP with colored noise**

Review of MAP

f_θ = *Family* of models, e.g., $f_\theta(x) = \theta^T x$

$$\hat{\theta} = \operatorname{argmax}_\theta \mathcal{L}(\theta; \mathcal{D})$$

MLE: $\mathcal{L}(\theta; \mathcal{D}) = p(\text{data} = \mathcal{D} \mid \text{model} = f_\theta)$

MAP: $\mathcal{L}(\theta; \mathcal{D}) = p(\text{model} = f_\theta \mid \text{data} = \mathcal{D})$

Review of MAP

$$\hat{\theta}_{\text{MLE}} = \arg \min_{\theta} -\log p(\text{data} = \mathcal{D} \mid \text{model} = f_{\theta})$$

$$\hat{\theta}_{\text{MAP}} = \arg \min_{\theta} \underbrace{-\log p(\text{data} = \mathcal{D} \mid \text{model} = f_{\theta})}_{\text{Same as MLE}} - \underbrace{\log p(\text{model} = f_{\theta})}_{\text{Prior}}$$

Same as MLE

Prior

Review of MAP

Assumption: $\theta^j \stackrel{iid}{\sim} \mathcal{N}(\mu_{\text{prior}}^j, \sigma_{\text{prior}}^2)$

$$\hat{\theta}_{\text{MAP}} = \arg \min_{\theta}$$

Review of MAP

Assumption: $\theta^j \stackrel{iid}{\sim} \mathcal{N}(\mu_{\text{prior}}^j, \sigma_{\text{prior}}^2)$

$$\hat{\theta}_{\text{MAP}} = \arg \min_{\theta} \sum_{i=1}^n (y_i - f_{\theta}(x_i))^2$$

Review of MAP

Assumption: $\theta^j \stackrel{iid}{\sim} \mathcal{N}(\mu_{\text{prior}}^j, \sigma_{\text{prior}}^2)$

$$\hat{\theta}_{\text{MAP}} = \arg \min_{\theta} \sum_{i=1}^n (y_i - f_{\theta}(x_i))^2 + \frac{\sigma^2}{\sigma_{\text{prior}}^2}$$

Review of MAP

Assumption: $\theta^j \stackrel{iid}{\sim} \mathcal{N}(\mu_{\text{prior}}^j, \sigma_{\text{prior}}^2)$

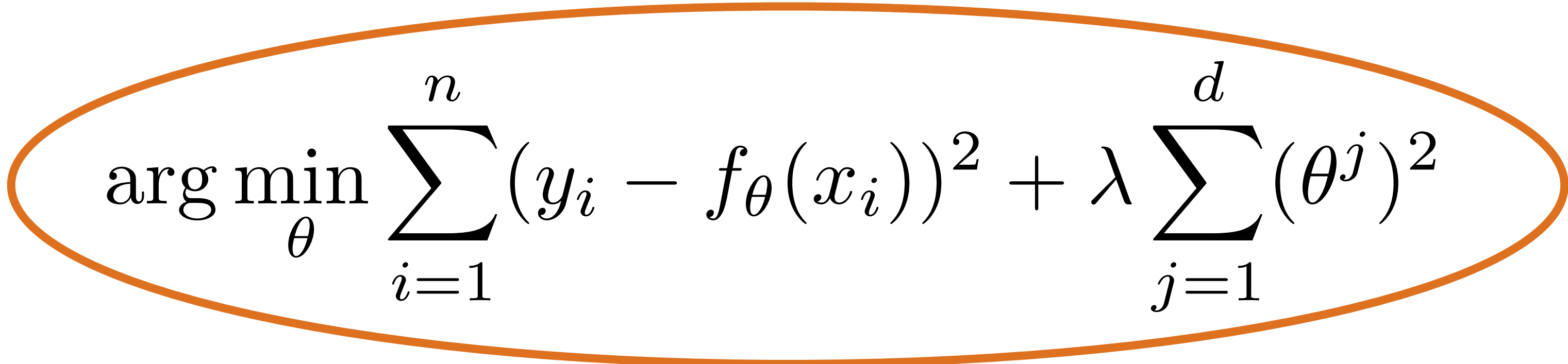
$$\hat{\theta}_{\text{MAP}} = \arg \min_{\theta} \sum_{i=1}^n (y_i - f_{\theta}(x_i))^2 + \frac{\sigma^2}{\sigma_{\text{prior}}^2} \sum_{j=1}^d (\theta^j - \mu_{\text{prior}}^j)^2$$

Review of MAP

Assumption: $\theta^j \stackrel{iid}{\sim} \mathcal{N}(\mu_{\text{prior}}^j, \sigma_{\text{prior}}^2)$

$$\hat{\theta}_{\text{MAP}} = \arg \min_{\theta} \sum_{i=1}^n (y_i - f_{\theta}(x_i))^2 + \frac{\sigma^2}{\sigma_{\text{prior}}^2} \sum_{j=1}^d (\theta^j - \mu_{\text{prior}}^j)^2$$

assume $\mu_{\text{prior}}^j = 0$ let $\lambda = \frac{\sigma^2}{\sigma_{\text{prior}}^2}$


$$\arg \min_{\theta} \sum_{i=1}^n (y_i - f_{\theta}(x_i))^2 + \lambda \sum_{j=1}^d (\theta^j)^2$$

Ridge regression

MAP with dependent parameters

Assumption: $\theta^j \stackrel{iid}{\sim} \mathcal{N}(\mu_{\text{prior}}^j, \sigma_{\text{prior}}^2)$

MAP with dependent parameters

~~Assumption: $\theta^j \stackrel{iid}{\sim} \mathcal{N}(\mu_{\text{prior}}^j, \sigma_{\text{prior}}^2)$~~

Assumption: $\theta \sim \mathcal{N}(\mu_{\theta}, \Sigma_{\theta})$

Can we transform back to the original problem?

MAP with dependent parameters

Probabilistic assumptions

$$\begin{array}{lll} y_i = f(\vec{x}_i) + z_i & \vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z) & \Sigma_z = \text{Any covariance matrix} \\ y_i = \vec{x}_i^T \theta + z_i & \theta \sim \mathcal{N}(\mu_\theta, \Sigma_\theta) & \end{array}$$

Derivation

$$\theta = \Sigma_\theta^{\frac{1}{2}} u + \mu_\theta \quad u \sim \mathcal{N}(0, I)$$

MAP with dependent parameters

Probabilistic assumptions

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Derivation

$$\theta = \Sigma_\theta^{-\frac{1}{2}} u + \mu_\theta \quad u \sim \mathcal{N}(0, I)$$

$$\vec{y} = X\theta + \vec{z}$$

MAP with dependent parameters

Probabilistic assumptions

$$\begin{array}{lll} y_i = f(\vec{x}_i) + z_i & \vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z) & \Sigma_z = \text{Any covariance matrix} \\ y_i = \vec{x}_i^T \theta + z_i & \theta \sim \mathcal{N}(\mu_\theta, \Sigma_\theta) & \end{array}$$

Derivation

$$\theta = \Sigma_\theta^{\frac{1}{2}} u + \mu_\theta \quad u \sim \mathcal{N}(0, I)$$

$$\vec{y} = X\theta + \vec{z} \implies \vec{y} = X \left(\Sigma_\theta^{\frac{1}{2}} u + \mu_\theta \right) + \vec{z}$$

MAP with dependent parameters

Probabilistic assumptions

$$y_i = f(\vec{x}_i) + z_i$$

$$\vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z)$$

$\Sigma_z =$ Any covariance matrix

$$y_i = \vec{x}_i^T \theta + z_i$$

$$\theta \sim \mathcal{N}(\mu_\theta, \Sigma_\theta)$$

$$\theta = \Sigma_\theta^{\frac{1}{2}} u + \mu_\theta \quad u \sim \mathcal{N}(0, I)$$

Derivation

$$\theta = \Sigma_\theta^{\frac{1}{2}} u + \mu_\theta \quad u \sim \mathcal{N}(0, I)$$

$$\begin{aligned} \vec{y} = X\theta + \vec{z} &\implies \vec{y} = X \left(\Sigma_\theta^{\frac{1}{2}} u + \mu_\theta \right) + \vec{z} \\ &\implies \vec{y} - X\mu_\theta = X\Sigma_\theta^{\frac{1}{2}} u + \vec{z} \end{aligned}$$

MAP with dependent parameters

Probabilistic assumptions

$$y_i = f(\vec{x}_i) + z_i$$

$$\vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z)$$

$\Sigma_z =$ Any covariance matrix

$$y_i = \vec{x}_i^T \theta + z_i$$

$$\theta \sim \mathcal{N}(\mu_\theta, \Sigma_\theta)$$

$$\theta = \Sigma_\theta^{\frac{1}{2}} u + \mu_\theta \quad u \sim \mathcal{N}(0, I)$$

Derivation

$$\underbrace{\vec{y} - X\mu_\theta}_{\tilde{y}} = \underbrace{\left(X\Sigma_\theta^{\frac{1}{2}}\right)}_{\tilde{X}} u + \vec{z}$$

$$\tilde{y} = \tilde{X}u + \vec{z}$$

Standard ridge regression with $\lambda = 1$

MAP with dependent parameters

Probabilistic assumptions

$$y_i = f(\vec{x}_i) + z_i$$

$$\vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z)$$

$\Sigma_z =$ Any covariance matrix

$$y_i = \vec{x}_i^T \theta + z_i$$

$$\theta \sim \mathcal{N}(\mu_\theta, \Sigma_\theta)$$

$$\theta = \Sigma_\theta^{\frac{1}{2}} u + \mu_\theta \quad u \sim \mathcal{N}(0, I)$$

Derivation

$$\vec{y} - X\mu_\theta = \left(X\Sigma_\theta^{\frac{1}{2}} \right) u + \vec{z}$$

$$\hat{u} = (\tilde{X}^T \tilde{X} + I)^{-1} \tilde{X}^T \tilde{y}$$

$\tilde{y}$

$\tilde{X}$

$$\tilde{y} = \tilde{X}u + \vec{z}$$

MAP with dependent parameters

Probabilistic assumptions

$$y_i = f(\vec{x}_i) + z_i$$

$$\vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z)$$

$\Sigma_z =$ Any covariance matrix

$$y_i = \vec{x}_i^T \theta + z_i$$

$$\theta \sim \mathcal{N}(\mu_\theta, \Sigma_\theta)$$

$$\theta = \Sigma_\theta^{\frac{1}{2}} u + \mu_\theta \quad u \sim \mathcal{N}(0, I)$$

Derivation

$$\vec{y} - X\mu_\theta = \left(X\Sigma_\theta^{\frac{1}{2}} \right) u + \vec{z}$$

$$\hat{u} = (\tilde{X}^T \tilde{X} + I)^{-1} \tilde{X}^T \tilde{y}$$

$\tilde{y}$

$\tilde{X}$

$\hat{u}$

MAP with dependent parameters

Probabilistic assumptions

$$y_i = f(\vec{x}_i) + z_i$$

$$\vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z)$$

$\Sigma_z =$ Any covariance matrix

$$y_i = \vec{x}_i^T \theta + z_i$$

$$\theta \sim \mathcal{N}(\mu_\theta, \Sigma_\theta)$$

$$\theta = \Sigma_\theta^{\frac{1}{2}} u + \mu_\theta \quad u \sim \mathcal{N}(0, I)$$

Derivation

$$\vec{y} - X\mu_\theta = \left(X \Sigma_\theta^{\frac{1}{2}} \right) u + \vec{z}$$

$$\hat{u} = (\tilde{X}^T \tilde{X} + I)^{-1} \tilde{X}^T \tilde{y}$$

$\tilde{y}$

$\tilde{X}$

$$\hat{u} = \left((\Sigma_\theta^{\frac{1}{2}})^T X^T X \Sigma_\theta^{\frac{1}{2}} + I \right)^{-1}$$

MAP with dependent parameters

Probabilistic assumptions

$$y_i = f(\vec{x}_i) + z_i$$

$$\vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z)$$

$\Sigma_z =$ Any covariance matrix

$$y_i = \vec{x}_i^T \theta + z_i$$

$$\theta \sim \mathcal{N}(\mu_\theta, \Sigma_\theta)$$

$$\theta = \Sigma_\theta^{\frac{1}{2}} u + \mu_\theta \quad u \sim \mathcal{N}(0, I)$$

Derivation

$$\vec{y} - X\mu_\theta = \left(X\Sigma_\theta^{\frac{1}{2}} \right) u + \vec{z}$$

$$\hat{u} = (\tilde{X}^T \tilde{X} + I)^{-1} \tilde{X}^T \tilde{y}$$

$\tilde{y}$

$\tilde{X}$

$$\hat{u} = \left((\Sigma_\theta^{\frac{1}{2}})^T X^T X \Sigma_\theta^{\frac{1}{2}} + I \right)^{-1} (\Sigma_\theta^{\frac{1}{2}})^T X^T$$

MAP with dependent parameters

Probabilistic assumptions

$$y_i = f(\vec{x}_i) + z_i$$

$$\vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z)$$

$\Sigma_z =$ Any covariance matrix

$$y_i = \vec{x}_i^T \theta + z_i$$

$$\theta \sim \mathcal{N}(\mu_\theta, \Sigma_\theta)$$

$$\theta = \Sigma_\theta^{\frac{1}{2}} u + \mu_\theta \quad u \sim \mathcal{N}(0, I)$$

Derivation

$$\vec{y} - X\mu_\theta = \left(X \Sigma_\theta^{\frac{1}{2}} \right) u + \vec{z}$$

$$\hat{u} = (\tilde{X}^T \tilde{X} + I)^{-1} \tilde{X}^T \tilde{y}$$

$\tilde{y}$

$\tilde{X}$

$$\hat{u} = \left((\Sigma_\theta^{\frac{1}{2}})^T X^T X \Sigma_\theta^{\frac{1}{2}} + I \right)^{-1} (\Sigma_\theta^{\frac{1}{2}})^T X^T (y - X\mu_\theta)$$

MAP with dependent parameters

Probabilistic assumptions

$$y_i = f(\vec{x}_i) + z_i$$

$$\vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z)$$

$\Sigma_z =$ Any covariance matrix

$$y_i = \vec{x}_i^T \theta + z_i$$

$$\theta \sim \mathcal{N}(\mu_\theta, \Sigma_\theta)$$

$$\theta = \Sigma_\theta^{\frac{1}{2}} u + \mu_\theta \quad u \sim \mathcal{N}(0, I)$$

Derivation

$$\hat{u} = \left((\Sigma_\theta^{\frac{1}{2}})^T X^T X \Sigma_\theta^{\frac{1}{2}} + I \right)^{-1} (\Sigma_\theta^{\frac{1}{2}})^T X^T (y - X \mu_\theta)$$

$$\hat{\theta} = \Sigma_\theta^{\frac{1}{2}} \hat{u} + \mu_\theta$$

MAP with dependent parameters

Probabilistic assumptions

$$y_i = f(\vec{x}_i) + z_i$$

$$\vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z)$$

$\Sigma_z =$ Any covariance matrix

$$y_i = \vec{x}_i^T \theta + z_i$$

$$\theta \sim \mathcal{N}(\mu_\theta, \Sigma_\theta)$$

$$\theta = \Sigma_\theta^{\frac{1}{2}} u + \mu_\theta \quad u \sim \mathcal{N}(0, I)$$

Derivation

$$\hat{u} = \left((\Sigma_\theta^{\frac{1}{2}})^T X^T X \Sigma_\theta^{\frac{1}{2}} + I \right)^{-1} (\Sigma_\theta^{\frac{1}{2}})^T X^T (y - X \mu_\theta)$$

$$\hat{\theta} = \Sigma_\theta^{\frac{1}{2}} \hat{u} + \mu_\theta$$

$$= \Sigma_\theta^{\frac{1}{2}} \left(\right.$$

MAP with dependent parameters

Probabilistic assumptions

$$y_i = f(\vec{x}_i) + z_i$$

$$\vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z)$$

$\Sigma_z =$ Any covariance matrix

$$y_i = \vec{x}_i^T \theta + z_i$$

$$\theta \sim \mathcal{N}(\mu_\theta, \Sigma_\theta)$$

$$\theta = \Sigma_\theta^{\frac{1}{2}} u + \mu_\theta \quad u \sim \mathcal{N}(0, I)$$

Derivation

$$\hat{u} = \left((\Sigma_\theta^{\frac{1}{2}})^T X^T X \Sigma_\theta^{\frac{1}{2}} + I \right)^{-1} (\Sigma_\theta^{\frac{1}{2}})^T X^T (y - X \mu_\theta)$$

$$\hat{\theta} = \Sigma_\theta^{\frac{1}{2}} \hat{u} + \mu_\theta$$

$$= \Sigma_\theta^{\frac{1}{2}} \left((\Sigma_\theta^{\frac{1}{2}})^T X^T X \Sigma_\theta^{\frac{1}{2}} + I \right)^{-1} (\Sigma_\theta^{\frac{1}{2}})^T X^T (y - X \mu_\theta)$$

MAP with dependent parameters

Probabilistic assumptions

$$\begin{aligned} y_i &= f(\vec{x}_i) + z_i & \vec{z} &\sim \mathcal{N}(\vec{0}, \Sigma_z) & \Sigma_z &= \text{Any covariance matrix} \\ y_i &= \vec{x}_i^T \theta + z_i & \theta &\sim \mathcal{N}(\mu_\theta, \Sigma_\theta) & \theta &= \Sigma_\theta^{\frac{1}{2}} u + \mu_\theta \quad u \sim \mathcal{N}(0, I) \end{aligned}$$

Derivation

$$\begin{aligned} \hat{u} &= \left((\Sigma_\theta^{\frac{1}{2}})^T X^T X \Sigma_\theta^{\frac{1}{2}} + I \right)^{-1} (\Sigma_\theta^{\frac{1}{2}})^T X^T (y - X \mu_\theta) \\ \hat{\theta} &= \Sigma_\theta^{\frac{1}{2}} \hat{u} + \mu_\theta \\ &= \Sigma_\theta^{\frac{1}{2}} \left((\Sigma_\theta^{\frac{1}{2}})^T X^T X \Sigma_\theta^{\frac{1}{2}} + I \right)^{-1} (\Sigma_\theta^{\frac{1}{2}})^T X^T (y - X \mu_\theta) + \mu_\theta \end{aligned}$$

MAP with dependent parameters

Probabilistic assumptions

$$y_i = f(\vec{x}_i) + z_i$$

$$\vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z)$$

$\Sigma_z =$ Any covariance matrix

$$y_i = \vec{x}_i^T \theta + z_i$$

$$\theta \sim \mathcal{N}(\mu_\theta, \Sigma_\theta)$$

$$\theta = \Sigma_\theta^{\frac{1}{2}} u + \mu_\theta \quad u \sim \mathcal{N}(0, I)$$

Derivation

$$\hat{u} = \left((\Sigma_\theta^{\frac{1}{2}})^T X^T X \Sigma_\theta^{\frac{1}{2}} + I \right)^{-1} (\Sigma_\theta^{\frac{1}{2}})^T X^T (y - X \mu_\theta)$$

$$\hat{\theta} = \Sigma_\theta^{\frac{1}{2}} \hat{u} + \mu_\theta$$

$$= \Sigma_\theta^{\frac{1}{2}} \left((\Sigma_\theta^{\frac{1}{2}})^T X^T X \Sigma_\theta^{\frac{1}{2}} + I \right)^{-1} (\Sigma_\theta^{\frac{1}{2}})^T X^T (y - X \mu_\theta) + \mu_\theta$$

MAP with dependent parameters

Probabilistic assumptions

$$y_i = f(\vec{x}_i) + z_i$$

$$\vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z)$$

$\Sigma_z =$ Any covariance matrix

$$y_i = \vec{x}_i^T \theta + z_i$$

$$\theta \sim \mathcal{N}(\mu_\theta, \Sigma_\theta)$$

$$\theta = \Sigma_\theta^{\frac{1}{2}} u + \mu_\theta \quad u \sim \mathcal{N}(0, I)$$

Derivation

$$\hat{\theta} = \cancel{\Sigma_\theta^{\frac{1}{2}}} \left((\Sigma_\theta^{\frac{1}{2}})^T X^T X \Sigma_\theta^{\frac{1}{2}} + I \right)^{-1} (\cancel{\Sigma_\theta^{\frac{1}{2}}})^T X^T (y - X \mu_\theta) + \mu_\theta$$

$$(\cancel{\Sigma_\theta^{\frac{1}{2}}})^T \left(X^T X + \underbrace{(\Sigma_\theta^{-\frac{1}{2}})^T \Sigma_\theta^{-\frac{1}{2}}}_{\downarrow \Sigma_\theta^{-1}} \right) \cancel{\Sigma_\theta^{\frac{1}{2}}}$$

$$\Sigma_\theta^{-1}$$

MAP with dependent parameters

Probabilistic assumptions

$$y_i = f(\vec{x}_i) + z_i$$

$$\vec{z} \sim \mathcal{N}(\vec{0}, \Sigma_z)$$

$\Sigma_z =$ Any covariance matrix

$$y_i = \vec{x}_i^T \theta + z_i$$

$$\theta \sim \mathcal{N}(\mu_\theta, \Sigma_\theta)$$

$$\theta = \Sigma_\theta^{\frac{1}{2}} u + \mu_\theta \quad u \sim \mathcal{N}(0, I)$$

Derivation

$$\begin{aligned} \hat{\theta} &= \Sigma_\theta^{\frac{1}{2}} \left((\Sigma_\theta^{\frac{1}{2}})^T X^T X \Sigma_\theta^{\frac{1}{2}} + I \right)^{-1} (\Sigma_\theta^{\frac{1}{2}})^T X^T (y - X \mu_\theta) + \mu_\theta \\ &= (X^T X + \Sigma_\theta^{-1})^{-1} X^T (y - X \mu_\theta) + \mu_\theta \end{aligned}$$

Summary of linear regression

MLE, iid noise

$$\hat{\theta}_{OLS} = (X^T X)^{-1} X^T y$$

MLE, MVG noise

$$\hat{\theta}_{GLS} = (X^T \Sigma_z^{-1} X)^{-1} X^T \Sigma_z^{-1} y$$

MAP, iid noise and parameters

$$\hat{\theta}_{\text{ridge}} = (X^T X + \lambda I)^{-1} X^T y$$

MAP, iid noise, MVG parameters

$$\hat{\theta}_{\text{MAP}} = (X^T X + \Sigma_{\theta}^{-1})^{-1} X^T (y - X \mu_{\theta}) + \mu_{\theta}$$

MAP, MVG noise, MVG parameters

$$\hat{\theta}_{\text{GMAP}} = (X^T \Sigma_z^{-1} X + \Sigma_{\theta}^{-1})^{-1} X^T \Sigma_z^{-1} y$$