Machine Learning for Regression

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Regression

Regression is an effort to describe the relationship between the response variable Y and p predictor variables (p features) $x_1, x_2, \ldots, x_p$.

Example: Modeling relationship between distance modulus (Y) and redshift for Type Ia Supernovae (x_1) is helpful for understanding different astrophysical theories (e.g., ΛCDM).

Example: Modeling relationship between Y (redshift) and $\{x_1, x_2, x_3, x_4, x_5\}$ (magnitudes in u, g, r, i, z bands) from photometry is essential for LSST and other photometric surveys.

Linear Regression

Linear Regression describes the relationship by a linear model.

Example: For the i-th object,

$$Y_i = \beta_0 + \beta_1 x_{i1} + \epsilon_i, \quad \epsilon_i \sim N(0,\ \sigma^2)$$

redshift

↳ dist. module

Example: For the i-th object,

$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_5 x_{i5} + \epsilon_i, \quad \epsilon_i \sim N(0,\ \sigma^2)$$

redshift x_{i1} u x_{i2} g x_{i5} z

Unifying matrix notation for any linear regression model:

$$Y_i = \begin{pmatrix} 1 & x_{i1} & x_{i2} & \cdots & x_{ip} \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{pmatrix} + \epsilon_i = x_i^T \beta + \epsilon_i$$

$$\begin{pmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{pmatrix}_{Y_{n\times 1}} = \begin{pmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1p} \\ 1 & x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{np} \end{pmatrix}_{X_{n\times(p+1)}} \begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{pmatrix}_{\beta_{(p+1)\times 1}} + \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{pmatrix}_{\epsilon_{n\times 1}}$$

$\epsilon \sim N_n(0, \Sigma)$ — a vector of zeros

↳ $\sigma^2 I_n$

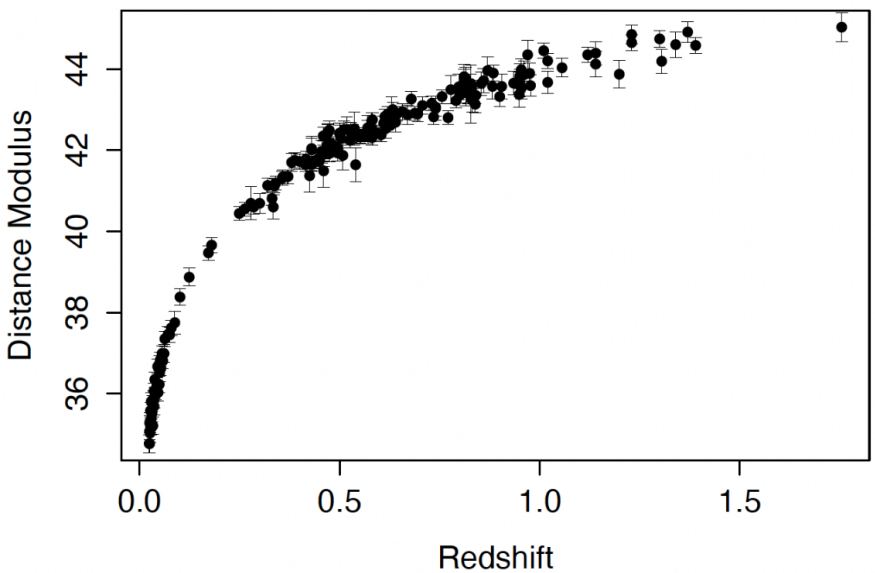
n-dim. multivariate Normal

Linear regression: Meaning of linearity

Linearity in a linear model means that $E(Y)$ is explained by a linear function of the regression coefficients β. That means, a model is linear as long as it is expressed as $E(Y) = X\beta$

Example: Learning the relationship between redshift and distance module can constrain Ω_m and H_0 under the ΛCDM (Riess et al., 2007).

DM



$$DM_i = \beta_0 + \beta_1 Red_i + \beta_2 Red_i^2 + \varepsilon_i$$

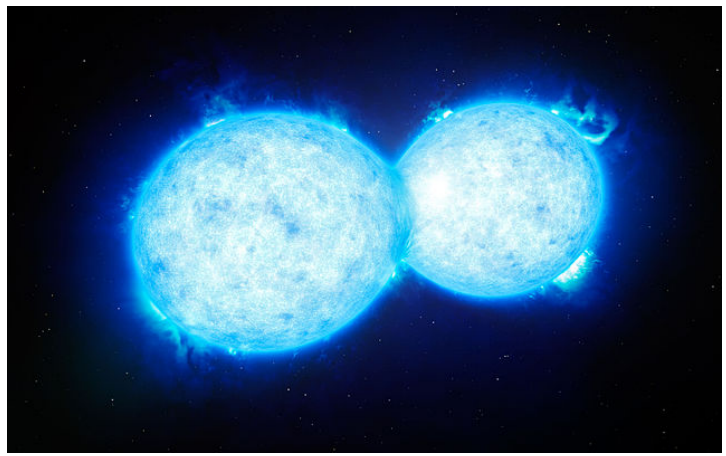
$$Y = X\beta + \varepsilon$$

$$= \begin{pmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ \vdots & \vdots & \vdots \\ 1 & x_n & x_n^2 \end{pmatrix} \beta + \varepsilon$$

Thus, a non-linear (quadratic) relationship between DM and redshift is being described by a linear model.

Linear regression: Meaning of linearity (cont.)

Example: The period-luminosity-color relation in early-type contact and near-contact binary stars.



The mathematical formulation of the period-luminosity-color relation (e.g., Pawlak, 2016; Almeida et al., 2015; Rucinski, 2004) is usually stated as

$$M_V = \beta_0 + \beta_1 \log(P) + \beta_2 (V - I)_0,$$

where M_V is the absolute V-band magnitude, P denotes the period and $(V - I)_0$ is the color between the filters V and I.

$= \log \frac{F_V}{F_I}$

Still within a linear model $Y = X\beta + \varepsilon$

Linear Regression: Maximum likelihood

Log-likelihood function of the model parameters, $\theta = (\beta, \Sigma)$, is used to infer the most likelihood values of θ, i.e., maximum likelihood estimates

$$\hat{\theta}_{MLE} = \arg\max_{\theta} \ \ell(\theta), \quad \text{where}$$

$$\ell(\theta) = \ln(L(\theta)) = c - \frac{1}{2}\ln(|\Sigma|) - \frac{1}{2}(y - X\beta)^\top \Sigma^{-1}(y - X\beta)$$

In machine learning, people typically infer θ as values that minimize a quadratic loss function. For example, least square estimates for β are the values that minimize a quadratic loss function:

$$\hat{\beta}_{LS} = \arg\min_{\beta} \ (y - X^\top \beta)^\top \Sigma^{-1}(y - X\beta)$$

Note: The two approaches are equivalent because maximizing $\ell(\theta)$ is equivalent to minimizing $-\ell(\theta)$.

$$\hat{\beta}_{MLE} = \arg\max_{\beta} \ \ell(\theta) = \hat{\beta}_{LS} = \arg\min_{\beta} \ [-\ell(\theta)]$$

Advanced regression modeling in astronomy

1. More general measurement error covariance matrices in a linear model.

Example: In astronomy, (1) most measurement data accompany 'completely known heteroscedastic measurement error uncertainties', and (2) response variables Y are not always independently measured, e.g., light curves.

2. Generalized linear models (non-linear models).

Example: In astronomy, response variables Y are not always Gaussian, e.g., Poisson counts and binary values.

3. Multi-output (multivariate) regression model.

Example: In astronomy, response variables Y can be vector-valued, e.g., multi-band light curves.

More general covariance matrices

Most astronomical data come with completely known heteroscedastic measurement error uncertainties.

The simplest scenario is to assume that X is measured without error (though not the case in astronomy; see Kelly (2007)) but only Y comes with the known heteroscedastic measurement error uncertainties.

Example: A weighted linear regression. Typical astronomical data are

Obs. number	Response Y redshift	Y's 1σ uncertainty	Features X u	g	r	i	z
1	y_1	σ_1	x_{11}	x_{12}	$\cdots$	$\cdots$	x_{15}
2	y_2	σ_2	x_{21}	x_{22}	$\cdots$	$\cdots$	x_{25}
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$			$\vdots$
n	y_n	σ_n	x_{n1}	x_{n2}	$\cdots$	$\cdots$	x_{n5}

More general covariance matrices (cont.)

Example (cont.): For the i-th object,

$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_5 x_{i5} + \epsilon_i, \quad \epsilon_i \sim N(0, w_i \sigma^2)$$

$w_i \to \frac{1}{\sigma_i^2}$

In matrix notation,

$$Y = X\beta + \varepsilon, \quad \varepsilon \sim N_n(0, \Sigma)$$

$$\Sigma = \sigma^2 \begin{pmatrix} w_1 & & 0 \\ & w_2 & \\ 0 & & \ddots \\ & & & w_n \end{pmatrix}$$

scalar

n-dim. diagonal matrix

Computationally, the model is still manageable because Σ is diagonal, and Σ^{-1} is easy to compute with $O(n)$ cost.

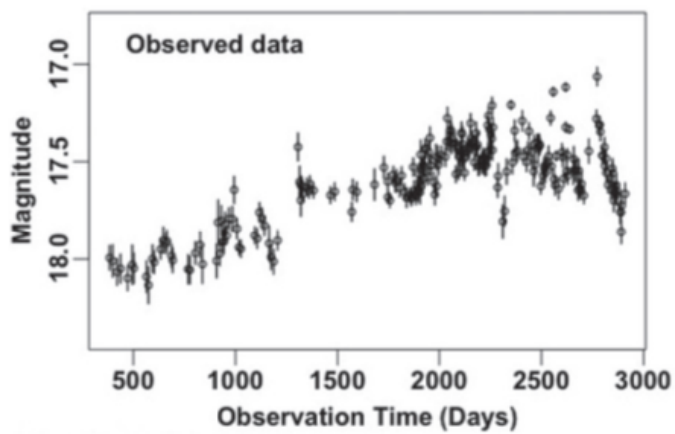
$$= \begin{pmatrix} 1/w_1 & & 0 \\ & 1/w_2 & \\ 0 & & \ddots \\ & & & 1/w_n \end{pmatrix}$$

More general covariance matrices (cont.)

In astronomy, response variables Y aren't always measured independently. Often, they are dependent, e.g., time-dependent structure in light curves.

Example: A Gaussian Process (GP) regression. Typical astronomical data for a single-band light curve are

Obs. number	Obs. time	Response Y mag.	Y's 1σ uncertainty
1	t_1	y_1	σ_1
2	t_2	y_2	σ_2
⋮	⋮	⋮	
n	t_n	y_n	σ_n



More general covariance matrices (cont.)

Example (cont.): The (time-)dependence among $Y = (Y_1, Y_2, \ldots, Y_n)$ is modeled by a non-diagonal covariance matrix Σ.

In matrix notation, $Y = X\beta + \varepsilon = \begin{pmatrix} \beta_0 \\ \beta_0 \\ \vdots \\ \beta_0 \end{pmatrix} + \varepsilon, \quad \varepsilon \sim N_n(0, \Sigma)$

→ overall avg. mag. β_0 (unknown)

$$\Sigma = \begin{pmatrix} \sigma_1^2 & & 0 \\ & \sigma_2^2 & \\ 0 & & \ddots \\ & & & \sigma_n^2 \end{pmatrix} + \begin{pmatrix} \Sigma_{11} & \Sigma_{12} & \cdots & \Sigma_{1n} \\ \Sigma_{21} & \Sigma_{22} & \cdots & \Sigma_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ \Sigma_{n1} & \Sigma_{n2} & \cdots & \Sigma_{nn} \end{pmatrix}$$

measurement error component (known)

time-dep. component → $\frac{n(n+1)}{2}$ unknowns too many?

Ex. Matérn ($\frac{1}{2}$) kernel (damped random walk process)

$\Sigma_{ij} = \sigma^2 \exp\left(-\frac{|t_i - t_j|}{\tau}\right)$, now just two unknowns, (σ^2, τ)

The computational cost for computing $\ell(\theta)$ is now prohibitive because Σ^{-1} in $\ell(\theta)$ involves $O(n^3)$ cost.

More general covariance matrices (cont.)

To overcome the daunting computational cost, astronomers have come up with computationally scalable GP models with $O(n^3) \to O(n)$.

Example: Kalman-filtering for CARMA(p, q)-type dependence structure (Kelly et al., 2014). It converts a computation of n-dim. multivariate Gaussian density to a multiplication of n univariate Gaussian densities.

$$L(\beta, \Sigma) = f(y_1, y_2, \ldots, y_n \mid \beta, \Sigma)$$

→ n-dim. MVN density with Σ^{-1}, culprit of $O(n^3)$

$$\overset{\text{KF}}{=} f_1(y_1 \mid \beta, \Sigma)\, f_2(y_2 \mid D_2, \beta, \Sigma) \cdots f_n(y_n \mid D_n, \beta, \Sigma)$$

$$D_i = (y_1, y_2, \ldots, y_{i-1})$$

A product of n univariate Gauss. densities, $O(n)$

Example: Other well-known scalable GP methods in astronomy are (but not limited to) celerite, S+LEAF, Quasi-separable kernels, etc.

Generalized linear models (GLMs)

In astronomy, response variables Y are not always modeled by Gaussian. For example, $Y_1, \ldots, Y_n$ may be integers like Poisson counts or binaries.

Example: Harris et al. (2013) study how the globular cluster population size is correlated somehow with global host galaxy properties. Their catalog data look as follows.

Obs. number	ID	Response Y	Features X		
		N_{GC}	M_V	logMd	logMGC
1	MilkyWay	160	-21.30	9.856	7.66
2	NGC7814	150	-20.18	10.879	7.57
⋮	⋮	⋮	⋮		⋮
256	NGC7768	3000	-23.07	12.142	9.04

Here N_{GC} is a measurement of globular cluster (GC) population size, M_V is the host galaxy visual magnitude in V-band, logMd is dynamical mass of the galaxy on a log scale, and logMGC is total stellar mass contained in the entire GC population of the galaxy on a log scale.

GLMs (cont.)

Can we still use a linear model in this case?

A linear model assumes that response variables Y are Gaussian random variables, meaning that each of Y is assumed to be real-valued on $\mathbb{R}$. But Y here are count data, meaning that each of Y here is integer-valued on $\{0, 1, \ldots\}$. That is, a Gaussian assumption on Y is not quite correct here.

We can still use a linear model, assuming that N_{GC} are Poisson counts, because Poisson counts can be approximated by Gaussian (central limit theorem). But this Gaussian approx. is accurate only for large N_{GC}.

A generalized linear model is a unified framework to relate a wide class of possible values of Y (including non-Gaussian cases) to features X. It provides a way to model N_{GC} as Poisson counts themselves w/o approx.

GLM: Poisson regression

Poisson regression (log-linear model) if $Y_i \in \{0, 1, 2, \ldots\} \sim \text{Pois}(\lambda_i)$

$$\log(\lambda_i) = x_i^\top \beta \quad \rightarrow \quad \lambda_i = \exp(x_i^\top \beta)$$

log is linear

That is,

$$Y_i \sim \text{Pois}(\exp(x_i^\top \beta)).$$

Example:

$$N_{GC,i} \sim \text{Pois}(\ \exp(\beta_0 + \beta_1 M_{V,i} + \beta_2 \log(Md_i) + \beta_3 \log(MGC_i))\ ).$$

Its likelihood function is

$$L(\beta) = \prod_{i=1}^{n} Pr(N_{GC,i} = y_i \mid \beta) = \prod_{i=1}^{n} \frac{\exp(x_i^\top \beta)^{y_i} \exp(-\exp(x_i^\top \beta))}{y_i!}.$$

Pois (λ_i) mass func. is $\frac{\lambda_i^{y_i} e^{-\lambda_i}}{y_i!}$

So, we can conduct a maximum likelihood estimation.

GLM: Poisson Regression (cont.)

R Output:

```
Call:
glm(formula = NGC ~ Mv + logMd + logMGC, family = poisson)

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-4.9820  -0.2255  -0.0857   0.1034   1.0430

Coefficients:
             Estimate Std. Error z value Pr(>|z|)
(Intercept) -9.570616   0.034900 -274.23   <2e-16 ***
Mv           0.139277   0.002972   46.86   <2e-16 ***
logMd       -0.001486   0.004791   -0.31    0.756
logMGC       2.301263   0.004550  505.81   <2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
```

Computation cost of glm in R: $O(p^3(1+n))$, where n = # of obs. and p = # of features

GLM: Logistic Regression

Binary variables are ubiquitous because it is always possible to make an indicator variable for any event of interest. $Y = \begin{cases} 1, & \text{high-}z \text{ quasars} \\ 0, & \text{otherwise} \end{cases}$

Example: Suppose we have an access to five colors (features) for each of 649,439 objects (20,640 high-z quasars, and 628,799 non-high-z quasars).

Obs. number	Response Y (binary)	Features X					
		ug	*gr*	*ri*	*iz*	*zs*1	*s*1*s*2
1	0	0.295	0.073	···	···	···	0.408
2	0	0.173	-0.035	···	···	···	0.299
⋮	⋮	⋮	⋮				⋮
649439	1	1.687	0.316	···	···	···	-0.161

GLM: Logistic Regression (cont.)

Logistic regression if $Y_i \in \{0, 1\} \sim \text{Bernoulli}(\theta_i)$

$$\log\left(\frac{\theta_i}{1-\theta_i}\right) = x_i^\top \beta \quad \rightarrow \quad \theta_i = \frac{1}{1+\exp(-x_i^\top \beta)}$$

logit func. of θ_i

That is,

$$Y_i \sim \text{Bernoulli}\left(\frac{1}{1+\exp(-x_i^\top \beta)}\right).$$

logistic func. of β or Sigmoid func. of β

Its likelihood function is

$$L(\beta) = \prod_{i=1}^{n} Pr(Y_i = y_i \mid \beta) = \prod_{i=1}^{n} \left(\frac{1}{1+\exp(-x_i^\top \beta)}\right)^{y_i} \left(\frac{\exp(-x_i^\top \beta)}{1+\exp(-x_i^\top \beta)}\right)^{1-y_i}.$$

So, we can conduct a maximum likelihood estimation.

GLM: Logistic Regression (cont.)

For simplicity, a subset of the data (size 100,000) is used to fit the model.

R Output:

```
Call:
glm(formula = quasar.indicator ~ ug + gr + ri + iz + zs1 + s1s2
    family = "binomial")

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-8.4904   0.0171   0.0794   0.1644   4.7351

Coefficients:
             Estimate Std. Error z value Pr(>|z|)
(Intercept)  5.388339   0.058314  92.403   <2e-16 ***
ug          -2.589888   0.035814 -72.315   <2e-16 ***
gr          -0.513882   0.086635  -5.932    3e-09 ***
ri           6.708540   0.160201  41.876   <2e-16 ***
iz           3.817042   0.115019  33.186   <2e-16 ***
zs1         -0.004496   0.030778  -0.146    0.884
s1s2        -3.093086   0.099175 -31.188   <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Again, $O(p^3(1+n))$

Multi-output regression

In astronomy, response variables Y are sometimes vector-valued.

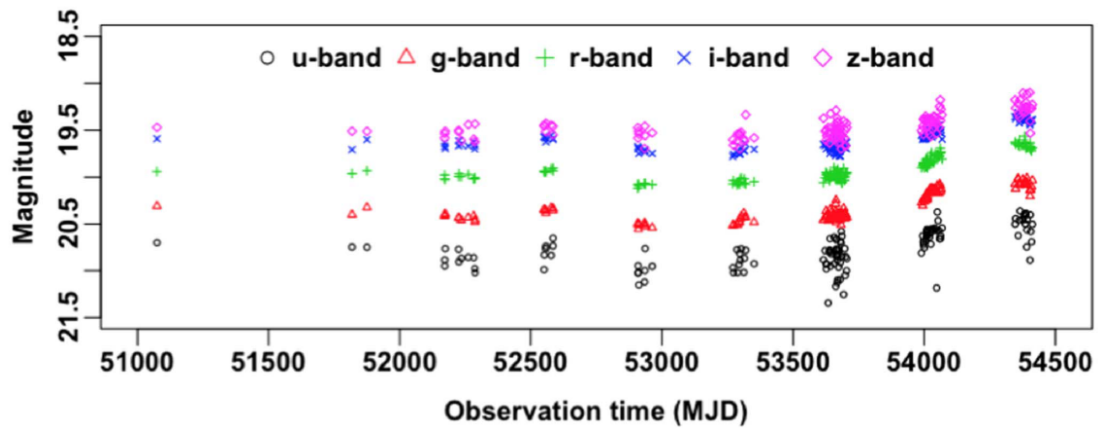
Example: A multi-output (vector-valued) Gaussian process regression. Typical astronomical data for multi-band light curves are

Obs. number	Obs. time	g-mag.	1σ error
1	t_1^g	y_1^g	σ_1^g
2	t_2^g	y_2^g	σ_2^g
$\vdots$	$\vdots$	$\vdots$	$\vdots$
n_g	$t_{n_g}^g$	$y_{n_g}^g$	$\sigma_{n_g}^g$

$\cdots$

Obs. number	Obs. time	r-mag.	1σ error
1	t_1^r	y_1^r	σ_1^r
2	t_2^r	y_2^r	σ_2^r
$\vdots$	$\vdots$	$\vdots$	$\vdots$
n_r	$t_{n_r}^r$	$y_{n_r}^r$	$\sigma_{n_r}^r$

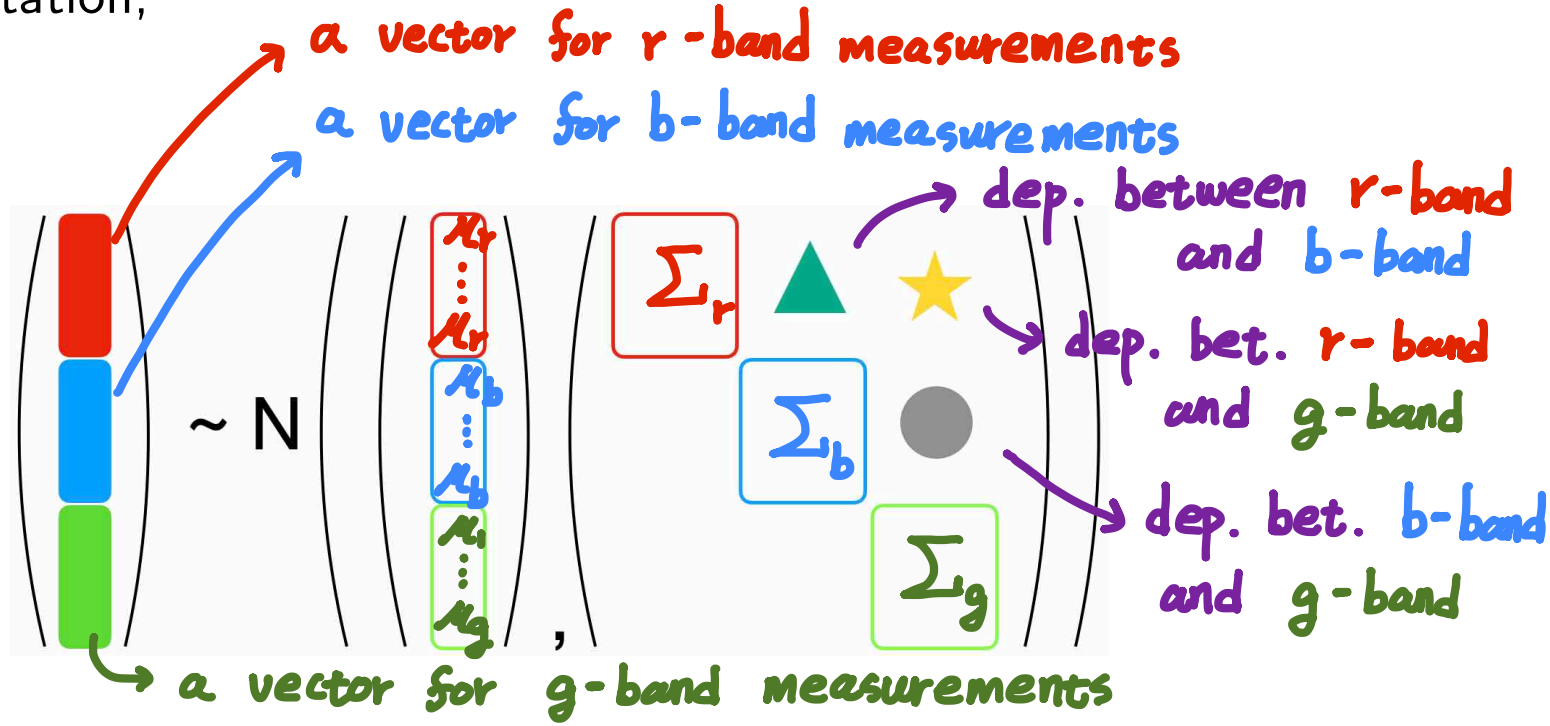
Five-band light curves of quasar 3078106 from a catalog of SDSS S82.



Multi-output regression (cont.)

Example (cont.): Time- and band-dependance among $Y = (Y_r, Y_b, Y_g)$ is now modeled by a really big non-diagonal covariance matrix Σ.

In matrix notation,



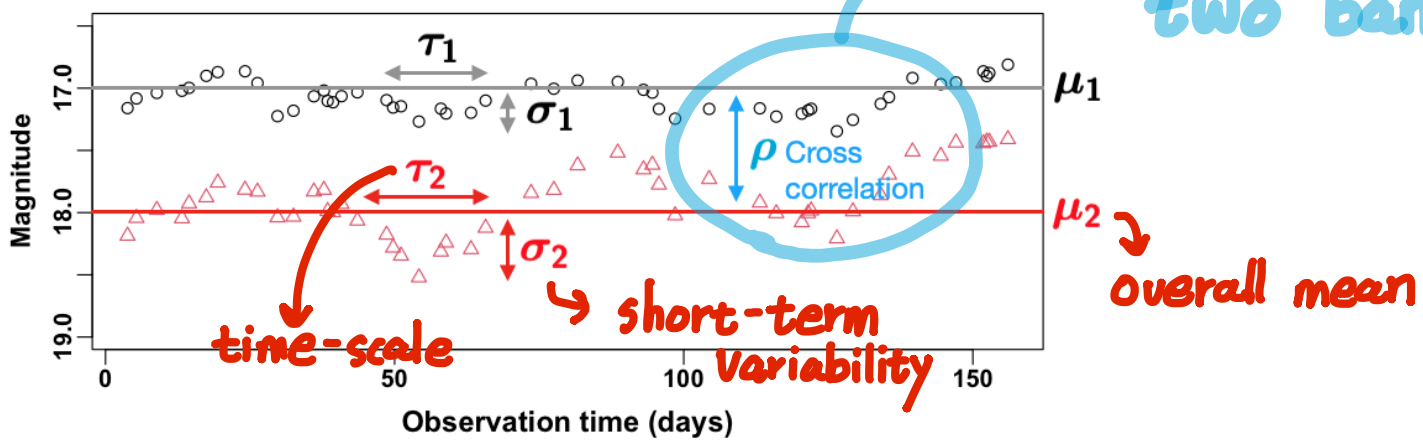
The computational cost for computing $\ell(\theta)$ is now even more prohibitive because Σ^{-1} in $\ell(\theta)$ involves $O((n_r + n_b + n_g)^3)$ cost.

Multi-output regression (cont.)

To overcome the daunting computational cost, astronomers have come up with computationally scalable Gaussian process models with

$$O((n_1 + n_2 + \cdots + n_5)^3) \to O(n_1 + n_2 + \cdots + n_5).$$

Example: Kalman-filtering for vectorized CARMA$(1, 0)$-type dependence structure (Hu and Tak, 2020).



θ, a vector of length 7 for two-band data
" 12 for three-band data