Triple-Gamma-Regularization

A Flexible Non-Convex Regularization Penalty based on the Triple-Gamma-Prior

Unterweger Lucas Paul

supervised by Peter Knaus, PhD

Vienna University of Econonomics and Business (WU), Department of Economics

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Overview

Motivating Problem

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What Is The Problem?

- **Sparse/High Dimensional Data Settings**: Scenarios where data is sparse, meaning the number of data points is limited relative to the number of features. Model is at risk of overfitting because the model can fit the noise than the underlying pattern.
- **Ill-posed Problems in Regression**: Solution to the problem becomes sensitive to small changes in the data, resulting in large variances in the estimated parameters.
- **Bias-Variance Tradeoff**: High variance models (*overfitting*) capture noise and fluctuations in training data $\implies$ poor generalization. High bias models (*underfitting*) can underestimate underlying effects. Hard to find balance!

A Visual Example

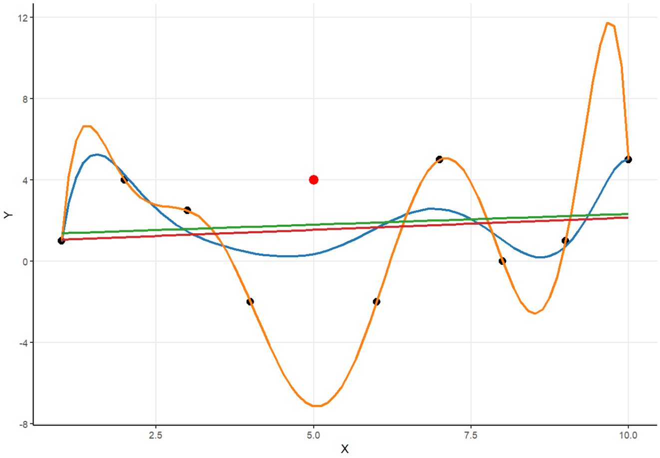

Figure 1: 1st and 8th order polynomial fit to data
(Green & Blue Lines fitted with red data point; Orange & Red Lines fitted without).

Some Solutions to Ill-posed Problems

1. **Cross-Validation** Estimate model based on subsets of the data to make estimates more robust. However, often not feasible due to data availablity issues.
2. **Feature Selection** Selecting a subset of relevant features, but often reliant on strict assumptions.
3. **Data Augmentation and Acquisition** Gather more data, use stochastic approaches to estimates your models, but similar issue as with *Cross-Validation*.
4. **Ensemble Methods** Combining the predictions of multiple models (e.g., bagging, boosting).
5. **Regularization using Loss Penalty** Induce shrinkage on esimates and penalize too-complex models by altering the Loss-function

Regularization

This thesis focuses on the 5th approach to *regularization*, which adds a penalty term to the risk minimization problem.

$$\min_{f \in \mathcal{H}} \left\{ \sum_{i=1}^{N} L(y_i, f_\beta(x_i)) + \lambda J(\beta) \right\}$$

where $L(.)$ refers to a loss function defined as some function of the true values y_i and the predicted values $f_\beta(x_i)$[1] and $J(\beta)$ is a penalty based on the chosen functional parameterized by β from a space of functions $\mathcal{H}$.

[1] In the setting of OLS, this would be the *sum of squared residuals (SSR)*

Regularization (LASSO)

This thesis focuses on the 5th approach to *regularization*, which adds a penalty term to the risk minimization problem.

$$\min_{f \in \mathcal{H}} \left\{ \frac{1}{N} \|y - X\beta\|_2^2 + \lambda \cdot \|\beta\|_1 \right\}$$

where $L(.)$ refers to a loss function defined as some function of the true values y_i and the predicted values $f(x_i)^2$ and $J(\beta)$ is a penalty based on the chosen functional parameterized by β from a space of functions $\mathcal{H}$.

[2] In the setting of OLS, this would be the *sum of squared residuals (SSR)*

Existing Concepts

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Established Concepts

Name	Penalty	Reference
Ridge	$\|\beta\|_2^2$	(Hoerl & Kennard, 1970)
LASSO	$\|\beta\|_1$	(Tibshirani, 1996)
Elastic Net	$\lambda_1 \|\beta\|_2^2 + \lambda_2 \|\beta\|_1$	(Zou & Hastie, 2005)
Arctan	$\frac{2}{\pi} \arctan(\lvert\beta\rvert)$	(Y. Wang & Zhu, 2016)
Gaussian	$1 - e^{-\beta^2}$	(John et al., 2022)

Table 1: Established Regularization Penalties

- others are *SCAD*, *MCP*, *SILO*, *Dantzig Selector*, ...
- F. Wang et al. (2020) find no "go-to" method which suits a broad range of problems

Motivating Duality of Ridge and LASSO

- An interesting mathematical connection can be found when looking at this problem from a Bayesian point of view.
- In Bayesian regression, the *posterior distribution* (up to a proportionality constant) takes the form

$$p(\beta|X,Y) \propto f(Y|X,\beta) \times p(\beta)$$

  with β being a coefficient vector, Y being the target vector and X being a matrix of features.
- Choosing specific prior distributions lead to posterior distributions which have moments that correspond to point estimates from regularization (*Gaussian prior*: Ridge; *double-exponential prior*: LASSO)

The Triple-Gamma-Prior

- Cadonna et al. (2020) developed a new prior distribution which has unifying properties and provides a general form for several shrinkage effects. Moreover, it is given by a closed-form solution[3]:

$$p(\beta_j|\phi^\xi, a^\xi, c^\xi) = \frac{\Gamma(c^\xi + \frac{1}{2})}{\sqrt{2\pi\phi^\xi} \cdot B(a^\xi, c^\xi)} \cdot U\left(c^\xi + \frac{1}{2}, \frac{3}{2} - a^\xi, \frac{\beta_j^2}{2\phi^\xi}\right)$$

Hypothesis/Aim of this thesis:

> *Can the closed-form marginal distribution of the Triple-Gamma-Prior be used to derive a new regularization penalty and do its advantages carry over into the frequentist framework?*

[3] Note that per definition $\phi^\xi = (2c^\xi)/(\kappa_B^2 a^\xi)$

Mathematical Derivation

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Likelihood

Let's assume we have n data points of a response variable $\mathbf{y}$ and and a set of features $\mathbf{X}$. Assuming a standard linear model with a parameter vector β and standard normal i.i.d. errors, the *likelihood* is

$$\begin{aligned}\mathcal{L}(\mathbf{y}|\beta,\sigma^2,\mathbf{X}) &= \prod_i^n p(y_i|\beta,\sigma^2,X_i)\\ &= \prod_i^n \frac{1}{\sqrt{2\pi\sigma^2}}\exp\left(-\frac{1}{2}\left(\frac{x_i-\mu}{\sigma}\right)^2\right)\\ &= \frac{1}{(2\pi\sigma^2)^{n/2}}\exp\left(-\frac{1}{2\sigma^2}\left\|\mathbf{y}-\mathbf{X}\beta\right\|_2^2\right)\end{aligned}$$

Prior

Assuming the individual parameters are independent a priori and using the *Triple-Gamma-Prior* from Cadonna et al. (2020), the *prior* distribution of the parameter vector β is

$$
\begin{aligned}
p(\beta) = \prod_j^p p(\beta_j) &= \prod_j^p p(\beta_j | \phi^\xi, a^\xi, c^\xi) \\
&\propto \prod_j^p U\left(c^\xi + \frac{1}{2}, \frac{3}{2} - a^\xi, \frac{\beta_j^2}{2\phi^\xi}\right) \\
&= \prod_j^p \frac{1}{\Gamma(c^\xi + \frac{1}{2})} \int_0^\infty e^{-(\frac{\beta_j^2}{2\phi^\xi})t} t^{c^\xi + \frac{1}{2} - 1} (1+t)^{\frac{3}{2} - a^\xi - c^\xi + \frac{1}{2} - 1} dt
\end{aligned}
$$

Posterior

Using Bayes' Theorem, the posterior distribution (up to a proportionality constant) $p(\beta|\mathbf{X}, \mathbf{y}, \sigma^2)$ is then given by

$$p(\beta|\mathbf{X}, \mathbf{y}, \sigma^2) \propto \mathcal{L}(\mathbf{y}|\beta, \sigma^2, \mathbf{X}) \times p(\beta)$$

Taking the $\log$ yields

$$\begin{aligned} \log(p(\beta|X, y, \sigma^2))) &\propto -\frac{1}{2\sigma^2} \|\mathbf{y} - \mathbf{X}\beta\|_2^2 + \log\left(\prod_j^p U\left(c^\xi + \frac{1}{2}, \frac{3}{2} - a^\xi, \frac{\beta_j^2}{2\phi^\xi}\right)\right) \\ &= -\frac{1}{2\sigma^2} \left\|\mathbf{y} - \mathbf{X}\beta^2\right\|_2^2 + \sum_j^p \log\left(U\left(c^\xi + \frac{1}{2}, \frac{3}{2} - a^\xi, \frac{\beta_j^2}{2\phi^\xi}\right)\right) \end{aligned}$$

Triple-Gamma-Regularization

Finally, the Triple-Gamma-Regularization can be retrieved from looking at the *maximum-a-posteriori* estimate, which minimizes the **negative**(!) log-posterior:

$$\hat{\beta}_{MAP} = \arg\min_{\beta \in \mathbb{R}^p} \left\{ \frac{1}{2\sigma^2} \|\mathbf{y} - \mathbf{X}\beta\|_2^2 + \lambda \cdot \sum_j^p - \log \left(U \left(c^\xi + \frac{1}{2}, \frac{3}{2} - a^\xi, \frac{\beta_j^2}{2\phi^\xi} \right) \right) \right\}$$

Thus, the **Triple-Gamma-Penalty** is given by:

$$J_{TGP}(\beta | a^\xi, c^\xi, \phi^\xi) = \sum_j^p - \log \left(U \left(c^\xi + \frac{1}{2}, \frac{3}{2} - a^\xi, \frac{\beta_j^2}{2\phi^\xi} \right) \right)$$

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Properties of the Triple-Gamma Penalty

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Comparison to other Penalties

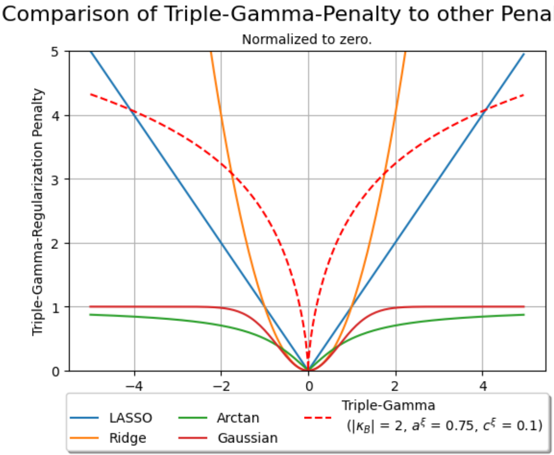
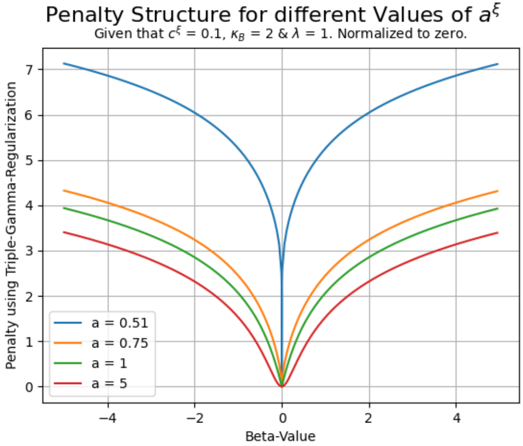


Figure 2: Comparison of one form of the Triple-Gamma-Penalty to existing penalties

Varying a^ξ


Penalty Structure for different Values of a^ξ
Given that $c^\xi = 0.1$, $\kappa_B = 2$ & $\lambda = 1$. Normalized to zero.
Penalty using Triple-Gamma-Regularization
Beta-Value
a = 0.51
a = 0.75
a = 1
a = 5
0
1
2
3
4
5
6
7
−4
−2
0
2
4

Varying c^ξ

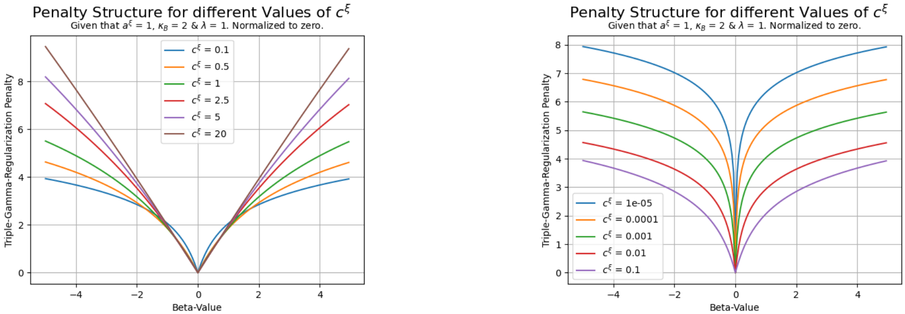
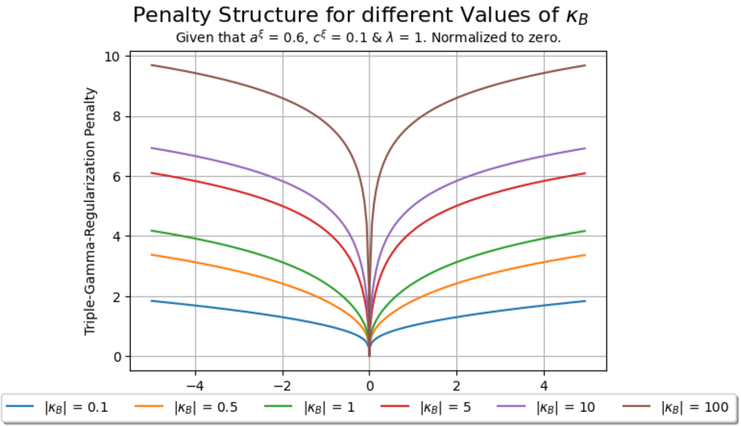


Figure 3: (Left) Varying $c^\xi \to \infty$, (Right) Varying $c^\xi \to 0$

Varying κ_B



Simulation Study

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Sparse Data Setting

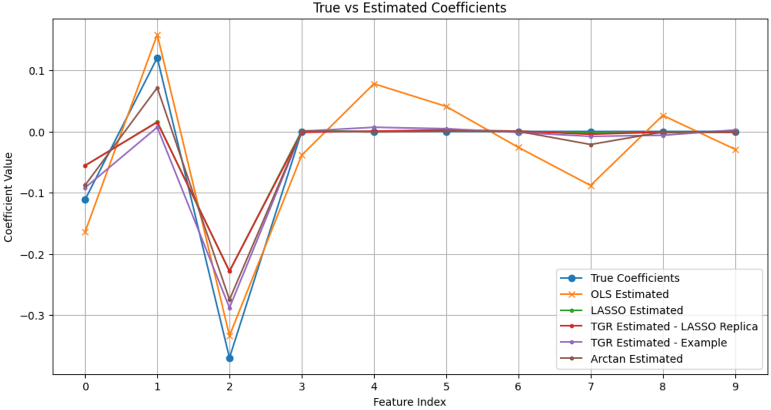

Figure 4: Comparison of Estimates from several Regularization Approaches $(n = 100, p = 10)$

Simulation Study

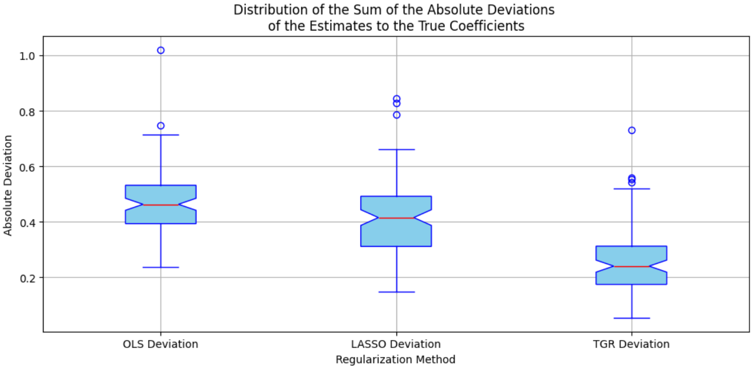

Figure 5: Distribution of the Sum of the Absolute Deviations of the Estimates to the True Coefficients (200 runs)

Shortcomings and Discussion

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Summary, Shortcomings & Potential Extensions

+ *Triple-Gamma-Penalty* is a flexible regularization penalty that corresponds with the Bayesian *Triple-Gamma-Prior*
+ It can replicate results from e.g. *LASSO* regression or induce its own form of shrinkage
+ Performs better in certain situations than existing penalties, but more testing and simulation needed

BUT

– Implementation in Python still relatively slow compared to similar approaches
– Cannot reproduce effects of converging non-convex penalties like *Arctan*, *Gaussian*, *etc* and mathematically not straight-forward

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Appendix

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Unifying Property of the Triple-Gamma-Prior

Table 1. Priors on $\sqrt{\theta_j}$ which are equivalent to (top) or special cases of (bottom) the triple gamma prior.

Prior for $\sqrt{\theta_j}$		a^ξ	c^ξ	κ_B^2	ϕ^ξ
$\mathcal{N}\left(0, \psi_j^2\right), \psi_j^2 \sim \mathrm{GG}\left(a^\xi, c^\xi, \phi^\xi\right)$	normal-gamma-gamma	a^ξ	c^ξ	$\frac{2c^\xi}{\phi^\xi a^\xi}$	ϕ^ξ
$\mathcal{N}\left(0, \frac{1}{\kappa_j}-1\right), \kappa_j \sim \mathcal{TPB}\left(a^\xi, c^\xi, \phi^\xi\right)$	generalized beta mixture	a^ξ	c^ξ	$\frac{2c^\xi}{\phi^\xi a^\xi}$	ϕ^ξ
$\mathcal{N}\left(0, \psi_j^2\right), \psi_j^2 \sim \mathrm{SBeta2}\left(a^\xi, c^\xi, \phi^\xi\right)$	hierarchical scaled beta2	a^ξ	c^ξ	$\frac{2c^\xi}{\phi^\xi a^\xi}$	ϕ^ξ
$\mathcal{DE}\left(0, \sqrt{2}\psi_j\right), \psi_j^2 \sim \mathcal{G}\left(c^\xi, \frac{1}{\lambda^2}\right)$	normal-exponential-gamma	1	c^ξ	$2\lambda^2 c^\xi$	$\frac{1}{\lambda^2}$
$\mathcal{N}\left(0, \tau^2\psi_j^2\right), \psi_j \sim t_1$	Horseshoe	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{2}{\tau^2}$	τ^2
$\mathcal{N}\left(0, \frac{1}{\kappa_j}-1\right), \kappa_j \sim \mathcal{B}(1/2, 1)$	Strawderman-Berger	$\frac{1}{2}$	1	4	1
$\mathcal{N}\left(0, \tau^2\tilde{\xi}_j\right), \tilde{\xi}_j \sim \mathcal{G}\left(a^\xi, a^\xi\right)$	double gamma	a^ξ	∞	$\frac{2}{\tau^2}$	-
$\mathcal{N}\left(0, \tau^2\tilde{\xi}_j\right), \tilde{\xi}_j \sim \mathcal{E}(1)$	Lasso	1	∞	$\frac{2}{\tau^2}$	-
$t_\nu\left(0, \tau^2\right)$	half-*t*	∞	$\frac{\nu}{2}$	$\frac{2}{\tau^2}$	-
$t_1\left(0, \tau^2\right)$	half-Cauchy	∞	$\frac{1}{2}$	$\frac{2}{\tau^2}$	-
$\mathcal{N}\left(0, B_0\right)$	normal	∞	∞	$\frac{2}{B_0}$	-

Figure 6: Table 1 from Cadonna et al. (2020)