

Practical Methods for Aggregating Banks' Economic Capital

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Abstract

This paper describes new procedures to aggregate banks' economic capital for commercial, retail, and market portfolios. It generalizes a result by calibrating the Gumbel copula through polynomials and provides a formula for estimating a three-dimensional copula. Consequently, two methods for aggregating risks are demonstrated and compared.

1. What Is Economic Capital?

Financial losses are not uncommon to banks. They are expected and, to certain extent, priced into the services. However, severe losses beyond the expectation (the “surprises”) will pose direct threats to banks' survivability. Banks often ask: What is the worst excessive loss the company can tolerate today? Banks' risk management often asks: What is the likelihood of such loss events in the future? Regulators put together both questions and ask: To ensure a high survivability (say, 99.9%) in the future, where should the bank set its loss tolerance level? This excessive loss level, and its associated survivability probability, is called economic capital (EC).

Technically EC is defined as follows: Suppose L_T is the total financial loss at time T . The time T is a prespecified time horizon (one year from today, for example). L_T is

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uncertain today and can represent any losses, ranging from the mildest to the most severe one. When a confidence level α is considered (say, $\alpha = 99.9\%$), EC is the loss level such that

$$Prob\{L_T \leq EC\} = \alpha, \text{ or equivalently,}$$

$$Prob\{L_T > EC\} = 1 - \alpha \text{ (which is } \frac{1}{1000} \text{ when } \alpha = 99.9\%)$$

In other words, EC is the capital level to absorb (up to) the worst yearly loss in 1,000 years.

2. Calculation of Economic Capital

Before explaining the ideas and methodologies, we start with a few challenges that make calculation of EC an unenjoyable and even frustrating process. The first is its all-inclusiveness. All risks, including credit risk, market risk, and operational risk, can threaten banks' survivability and therefore have to be included in the calculation. These risks are, however, not equally understood or managed by financial institutions. To assess their financial impacts with the same accuracy and the same confidence is very appealing but also thrilling. Because EC deals with rare loss events, to create severe event scenarios and to capture loss behaviors with little or no historical data is sometimes frustrating. With the numerous financial products a bank typically offers today, to develop distinctive techniques for risk evaluation at the product level is a daunting task. Even when all individual components are properly developed, putting all the pieces together to form a holistic view is no less complex. In fact, risk aggregation determines one of the biggest EC benefits: the diversification benefit for financial institutions. It is this benefit that drives banks' decision in adopting an EC approach.

The risk-based nature makes EC calculations performed mostly by risk types: credit risk, market risk and operational risk. Within credit risk, banks commonly build separate EC processes for a retail credit portfolio and a commercial credit portfolio because they exhibit distinctive risk behaviors and require different modeling techniques. The most common method for a commercial portfolio is to use a bottom-up approach where each obligor is modeled individually, and its risk parameters such as probability of default, loss given default, and exposure at default are estimated based on simulated economic scenarios. One key in this approach is the pairwise default correlation among different obligors. For retail portfolios, banks typically bucket the exposures based on risk characters such as FICO, coupon, maturity, collaterals, etc., and perform calculations at the bucket level. Market risk requires a price calculation for every instrument in the portfolio, and a multifactor modeling approach is standard because the prices are driven by market factors such as interest rates, volatilities, and credit spreads.

After losses are individually estimated for all risks, consolidating the outcomes in a coherent manner requires comprehensive understanding of risk interactions and development of necessary calibration techniques. In other words, knowing individual risks completely would not suffice to determine the loss at the enterprise level. Risk aggregation becomes the next challenge.

3. Approaches for Risk Aggregation

The ideal method is a direct simulation of all risks and their drivers including all the correlations. But this can hardly be practical because risks are driven by many different factors, and their relationship is difficult to be reliably captured and modeled. Another

method is to make direct distributional assumptions about the aggregated loss based on statistical limiting properties or historical loss experience. This approach is often criticized for being too judgmental because the statistical conditions are difficult to verify and historical experiences are generally not sufficiently severe. Banks sometimes try approximation methods such as Delta-Gamma, Cornish-Fisher, or Saddle Point. However, given the long time horizon (one year in general) considered by EC, such approximations can produce results that sometimes are less justifiable.

The most feasible and flexible approach seems to be the copula method. It separates the aggregation process from the risk-modeling process so that the underlying calculations can be performed independently. The method becomes particularly attractive when external data and experience have to be used as proxies.

4. Using a Copula for Risk Aggregation

The copula method is popular but not without concerns. It is fairly judgmental in the selection of the right copula, and its calibration method is generally complicated. We will explain at a later time our selection criteria and provide a simpler calibration method for the Gumbel copula based on the roots of polynomials. Our method will be demonstrated for aggregate retail, commercial, and market risks and compared with the sophisticated “Nested copula” approach.

4.1. Definition of Copula

A copula is a function that expresses a joint probability function as a function of marginal distributions:

A k -dimensional copula among random variables X_1, \dots, X_k is a function $C(u_1, \dots, u_k)$ from $[0,1]^k \rightarrow [0,1]$ such that

$$\text{Prob}\{X_1 \leq x_1, \dots, X_k \leq x_k\} = C(F_1(x_1), \dots, F_k(x_k)),$$

where $F_i(x) = \text{Prob}\{X_i \leq x_i\}$ is the cumulative distribution function for X_i .

A copula can capture any relationship among any random variables; this is demonstrated by the following powerful theorem of Sklar's.

4.1.1. Theorem (Sklar 1959) (See Nelsen, R.B.2006)

Let F be a k -dimensional cumulative distribution function with marginal distributions F_1, \dots, F_k . Then there is a copula function C such that

$$\text{Prob}\{X_1 \leq x_1, \dots, X_k \leq x_k\} = C(F_1(x_1), \dots, F_k(x_k)).$$

4.2. Selection of Copulae

There are many types of copulae, including the popular Gaussian and Student's t copula, the elliptical, and the Archimedean copulae.

The Gaussian copula has been widely used for its intuitive concept and easy calibration. It was introduced to price collateralized debt obligations and, unfortunately,

led to catastrophic consequences during the global financial crisis of 2008–2009. It is most commonly criticized for its lack of sensitivity to stressed situations.

The Archimedean copulae is a rich and well-understood class whose members include the Clayton, Gumbel, and Frank families. Each Archimedean copula is generated by a single “generator,” which makes it somewhat manageable, but the choice of the generators is nearly endless, as was demonstrated by this author’s published research in 1996 (Sungur and Yang 1996).

4.2.1. Definition

Let ϕ be a continuous, strictly decreasing, convex function from $[0, 1]$ to $[0, \infty)$ such that $\phi(1) = 0$, and let ϕ^{-1} be its pseudo-inverse, then $C(u_1, \dots, u_k) = \phi^{-1}(\phi(u_1) + \dots + \phi(u_k))$ is a k -dimensional Archimedean copula.

1) For the Clayton family, the generator is of the form $\phi(u) = \frac{u^{-\theta} - 1}{\theta}$ with parameter

$$\theta \in [-1, \infty) \setminus \{0\}.$$

2) For the Frank family, the generator is $\phi(u) = -\ln \frac{e^{-\theta u} - 1}{e^{-\theta} - 1}$ with $\theta \neq 0$.

3) For the Gumbel family, the generator is given by $\phi(u) = (-\ln u)^\theta$ with $\theta \geq 1$.

In order to aggregate losses, one needs to select an appropriate copula. Our selection is based on the following criteria: (1) It is sensitive to tail losses; that is, it has a so-called “fat tail.” (2) Ideally it should be more sensitive to large losses and less sensitive to small losses—in other words, its tail is one-sided. (3) Its parameter can be easily calibrated. (4) Finally, the implementation is simple.

4.2.2. Tails of Archimedean Copulae

Let C be the copula between random variables X and Y . Then its tail dependence is defined as

1) Upper tail dependence: $\lambda_U = 2 - \lim_{t \rightarrow 1^-} \frac{1 - C(t, t)}{1 - t}$.

2) Lower tail dependence: $\lambda_L = \lim_{t \rightarrow 0^+} \frac{C(t, t)}{t}$.

4.2.3. Proposition

1) For the Gaussian copula: $\lambda_L = 0$, and $\lambda_U = 0$.

2) For the Clayton copula: $\lambda_L = 2^{-\frac{1}{\theta}}$, and $\lambda_U = 0$. The copula has only a left tail.

3) For the Frank copula: $\lambda_L = 0$, and $\lambda_U = 0$. The copula has no tails.

4) For the Gumbel copula: $\lambda_L = 0$, and $\lambda_U = 2 - 2^{\frac{1}{\theta}}$. The copula has only a right tail.

It appears that among the aforementioned copulae, only the Gumbel family has a one-sided right tail. This can be seen from the following simulated graphs for Gaussian and Gumbel copulae (Figs. 1 and 2).

Figure 1: Gaussian Copula

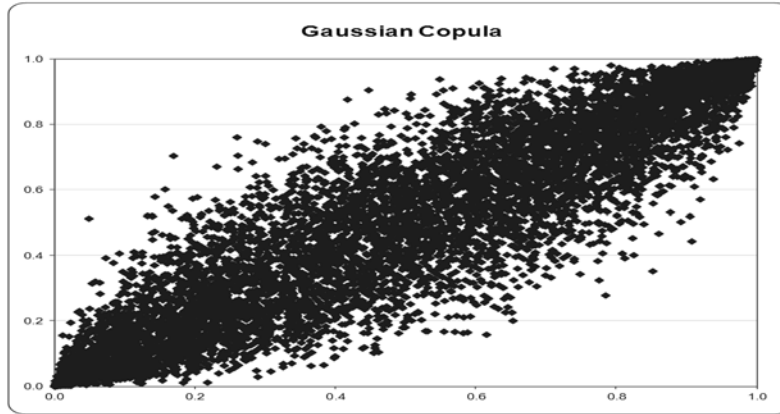
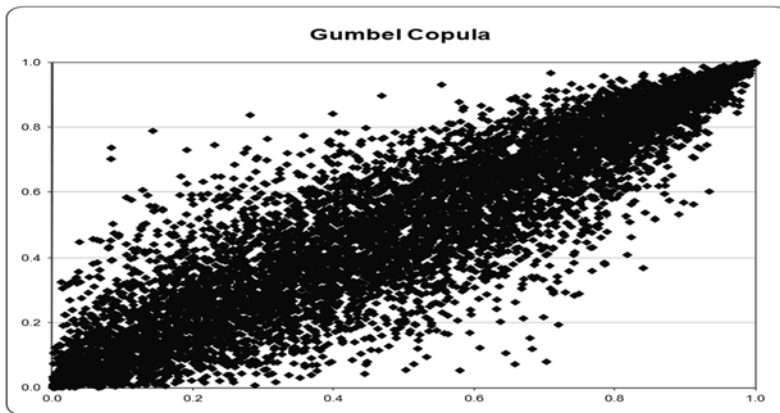


Figure 2: Gumbel Copula



In both figures, the x and y axes exhibit the loss severity percentiles for the two random variables (the higher, the worse) with the diagonal line representing the correlation. For the Gaussian copula, both ends display similar patterns. But for the Gumbel copula, the sharper upper-right corner indicates a higher correlation. This justifies our use of the Gumbel copula for EC aggregation.

5. Results

Before we state our results, we introduce a few statistical concepts.

5.1. Definition (Cumulative K-function):

Suppose U_1, \dots, U_k are uniform variables whose joint distribution is given by a k -dimensional Archimedean copula C . Let $W = C(U_1, \dots, U_k)$ and define the cumulative K function as $K(t) = \text{Prob}\{W \leq t\}$.

5.1.1. Proposition

Let ϕ be the generator of Archimedean copula C , then

$$K(t) = t + \sum_{i=1}^{k-1} (-1)^i \frac{\{\phi(t)\}^i}{i!} \frac{d^i}{dx^i} \phi^{-1}(x) \Big|_{x=\phi(t)}.$$

5.1.2. Empirical Estimation of the K Function

If we have empirically observed the random vector $U = (U_1, \dots, U_k)$, then the K function can be estimated through the following procedure:

Let $\{U_i = (U_{1i}, \dots, U_{ki})\}_{i=1, \dots, n}$ be n independent observations. Define:

$$W_j = \frac{1}{n} \sum_{i=1}^n \mathbf{1}_{(U_{1i} \leq U_{1j}, \dots, U_{ki} \leq U_{kj})} = \frac{\{\text{Number of } U_i = (U_{1i}, \dots, U_{ki}) \text{ such that } U_{1i} \leq U_{1j}, \dots, U_{ki} \leq U_{kj}\}}{n}$$

where $\mathbf{1}_{(U_{1i} \leq U_{1j}, \dots, U_{ki} \leq U_{kj})}$ is the indicating function. Let

$$\hat{K}(t) = \frac{1}{n} \sum_{i=1}^n \mathbf{1}_{(W_i \leq t)} = \frac{\text{Number of } W_i \text{ such that } W_i \leq t}{n}.$$

Then $\hat{K}(t)$ is an empirical estimation for $K(t)$.

Now we can summarize our results below. The proof is provided in the Appendix.

5.2. Proposition (Gumbel Copula Parameter Estimation)

Suppose C is a k -dimensional Gumbel copula with parameter θ and $z = \frac{1}{\theta}$. Assume

$\{w_j\}_{j=1, \dots, n}$ defined above has Q distinct values: $\{w_1^* < w_2^* < \dots < w_Q^*\}$. Let n_i be the

multiplicity of w_i^* and $k_i = \frac{\sum_{t=1}^i n_t}{n}$. Then

1) $K(t)$ is a polynomial of degree $k - 1$ in $z = \frac{1}{\theta}$. In fact, the terms in $K(t)$ can be

calculated using the following recursive formula:

$$\{\phi(t)\}^i \frac{d^i}{dx^i} \phi^{-1}(x) \Big|_{x=\phi(t)} = t \sum_{j=1}^i Q_j^i \cdot \ln^j t ;$$

$$Q_j^{i+1} = z Q_{j-1}^i + (z \cdot j - i) \cdot Q_j^i$$

with the convention that $Q_1^1 = z$ and $Q_j^i = 0$ for $j > i$ or $j \leq 0$.

2) The integral $\int_0^1 (K(t) - \hat{K}(t))^2 dt$ is a polynomial of degree $2(k - 1)$ in z . It has a

global minimal value for $z = \frac{1}{\theta}$ of some real root of its derivative polynomial (of degree $2k - 3$).

3) For $k = 2$, $\int_0^1 (K(t) - \hat{K}(t))^2 dt$ reaches its minimal value at $\theta = -\frac{4}{27 \cdot \alpha}$ for

$$\alpha = \frac{2}{9} + \sum_{i=1}^Q k_i \left\{ \left(\ln w_{i+1}^* - \frac{1}{2} \right) w_{i+1}^{*2} - \left(\ln w_i^* - \frac{1}{2} \right) w_i^{*2} \right\} \text{ with the convention that}$$

$$w_{Q+1}^* = 1.$$

4) For $k = 3$, $\int_0^1 (K(t) - \hat{K}(t))^2 dt$ reaches its minimal value at

$$\theta = \frac{1}{\sqrt[3]{-\frac{81\gamma}{4} + \sqrt{\frac{6561\gamma^2}{16} + \frac{19683\beta^3}{8}}} + \sqrt[3]{-\frac{81\gamma}{4} - \sqrt{\frac{6561\gamma^2}{16} + \frac{19683\beta^3}{8}}}} \quad \text{with}$$

$$\beta = \frac{7}{27} - \sum_{i=1}^Q k_i \{w_{i+1}^{*2} \ln^2 w_{i+1}^* - w_i^{*2} \ln^2 w_i^*\} \text{ and}$$

$$\gamma = \frac{1}{3} + \sum_{i=1}^Q k_i \left\{ \frac{3}{2} (w_{i+1}^{*2} \ln w_{i+1}^* - w_i^{*2} \ln w_i^*) - \frac{3}{4} (w_{i+1}^{*2} - w_i^{*2}) \right\}.$$

We will see examples of EC calculations using these estimations.

6. Economic Capital Calculation (Example I)

One advantage of using a copula is that it can be calibrated utilizing external data resources. Suppose we have three portfolios: a commercial credit portfolio, a retail credit portfolio (without credit card), and an investment portfolio. Without sufficient historical loss data, we will demonstrate how to use Fed data and the S&P500 index for its calibration.

6.1. Our Portfolios

Assume for the selected portfolios that we have already obtained their loss distributions through other processes. In fact, their EC values at various confidence levels are given as shown in Table 1.

Table 1

Portfolio EC/Loss Distribution

\$mm	Economic Capital			Total (Undiversified) EC	
Confidence	Commercial	Retail	Investment	Total Credit	ALL
99.00%	726	482	349	1,208	1,557
99.90%	1,179	741	464	1,920	2,383
99.99%	1,672	1,003	558	2,674	3,232

6.2. Fed Data

The Federal Reserve publishes bank loan loss data on a quarterly basis. Charge-off rates are available for both Commercial & Industry (C&I) loans and consumer loans. These loss experiences may quite different from our credit portfolios. However, the relationship and the risk interaction between C&I loans and consumer loans implied by the data can be adopted to fit our portfolios because the Fed's data was pulled from all banks. In fact, we will see that only the risk interaction (the copula), not the actual charge-offs, will be used in our calibration.

We use the following (partially listed) Fed quarterly charge-off data for 1985 to 2012.

Table 2**Fed Data**

Charge Off	Real estate loans				Consumer loans			Leases	C&I loans	Agricultural loans	Total loans and leases
	All	Booked in domestic offices			All	Credit cards	Other				
		Residential	Commercial	Farmloan							
2012:02	1.14	1.35	0.74	0.78	2.71	4.26	0.96	0.32	0.47	0.77	1.21
2012:01	1.29	1.55	0.80	0.37	2.82	4.38	1.05	0.11	0.48	0.39	1.32
2011:04	1.36	1.49	1.15	0.58	3.09	4.54	1.40	0.32	0.66	0.28	1.47
2011:03	1.51	1.66	1.29	0.60	3.68	5.67	1.34	0.17	0.68	0.28	1.66
2011:02	1.70	1.83	1.50	0.83	3.66	5.60	1.37	0.10	0.74	0.52	1.79
2011:01	1.77	1.88	1.64	1.08	4.68	6.99	1.84	0.16	1.08	1.06	2.14
2010:04	2.28	2.17	2.68	1.02	5.10	7.72	2.01	0.72	1.34	2.11	2.56
2010:03	2.28	2.12	2.80	0.83	5.56	8.59	1.94	0.47	1.74	1.98	2.78
2010:02	2.43	2.37	2.72	0.94	7.06	11.05	2.22	0.69	1.80	1.19	3.19
2010:01	2.65	2.75	2.50	0.77	6.94	10.20	2.65	0.82	2.00	2.86	3.36
2009:04	3.15	3.16	3.37	0.66	6.06	10.16	3.25	1.35	2.61	1.13	3.38
2009:03	2.66	2.72	2.74	0.63	6.12	10.32	3.33	1.36	2.65	0.96	3.14
2009:02	2.48	2.66	2.30	0.29	6.05	9.87	3.38	1.29	2.34	0.61	2.91
2009:01	1.81	2.06	1.44	0.16	5.11	7.65	3.25	0.71	1.81	0.50	2.28
2008:04	1.96	1.80	2.43	0.33	4.44	6.19	3.24	0.71	1.52	0.33	2.17
2008:03	1.49	1.66	1.28	0.06	3.69	5.55	2.52	0.52	0.97	0.28	1.65
2008:02	1.22	1.32	1.12	0.17	3.38	5.38	2.17	0.27	0.80	0.22	1.38
2008:01	0.80	0.96	0.52	0.09	3.09	4.63	2.08	0.31	0.64	0.08	1.09

6.3. Standard & Poor's 500 Index

Assume that our investment portfolio is sufficiently diversified. We do not have to assume that our portfolio follows the S&P500 index faithfully. Rather, we assume only that our investment portfolio resembles similar risk characteristics, so its relationship with the credit portfolios can be assessed.

To be consistent with the Fed data, we use the index's quarterly data. In fact, we will use index losses instead of returns. Taking the historical return average as the baseline (the choice of the baseline will not affect the fitting of the copula), we calculate losses below it.

It is known that credit loss is a lagging event following the market, and the data do indicate a five-quarter lag behind the S&P500 index. In Table 3 the lag is appropriately incorporated.

Table 3
S&P500 Index and Fed Data

	SP500 Loss %	Retail CO	C&I CO
2012:02	-3.19	0.96	0.47
2012:01	-7.97	1.05	0.48
2011:04	-8.49	1.40	0.66
2011:03	14.09	1.34	0.68
2011:02	-2.64	1.37	0.74
2011:01	-3.26	1.84	1.08
2010:04	-12.75	2.01	1.34
2010:03	-12.99	1.94	1.74
2010:02	13.90	2.22	1.80
2010:01	24.79	2.65	2.00
2009:04	11.11	3.25	2.61
2009:03	5.46	3.33	2.65
2009:02	12.15	3.38	2.34
2009:01	6.05	3.25	1.81
2008:04	0.67	3.24	1.52
2008:03	-3.58	2.52	0.97
2008:02	2.05	2.17	0.80
2008:01	-3.94	2.08	0.64

6.4. Fitting the Copula

To fit the copula, we use the following procedure:

- 1) *Generate uniform distributions from Fed and S&P500 data through percentile ranking*
- 2) *Calculate the parameter θ using Proposition 5.2*
- 3) *Simulate the joint copula*
- 4) *Apply the simulated copula to our portfolio loss distributions to calculate aggregated (diversified) EC.*

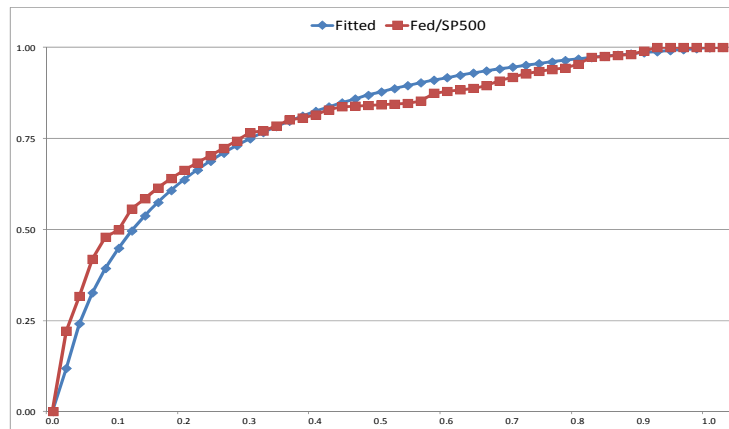
Following the procedure, we obtain the uniform distributions shown in Table 4.

Table 4

Uniform Distributions

PCT Ranking	SP500	Retail	C&I
2012:02	0.339	0.284	0.302
2012:01	0.128	0.339	0.311
2011:04	0.110	0.688	0.403
2011:03	0.935	0.633	0.422
2011:02	0.385	0.651	0.477
2011:01	0.330	0.853	0.642
2010:04	0.045	0.880	0.770
2010:03	0.036	0.871	0.871
2010:02	0.926	0.917	0.880
2010:01	0.990	0.954	0.935
2009:04	0.899	0.972	0.990
2009:03	0.798	0.990	1.000
2009:02	0.908	1.000	0.972
2009:01	0.844	0.972	0.889
2008:04	0.605	0.963	0.834
2008:03	0.302	0.944	0.614
2008:02	0.669	0.899	0.522
2008:01	0.284	0.889	0.385

Figure 3: Three-Dimensional Fitting with Parameter $\theta = 1.247829641$



Several available algorithms can be used to simulate a three-dimensional Gumbel copula. Based on our simulation and the portfolio loss distributions, the diversified EC is calculated as shown in Table 5.

Table 5

Total (Aggregated) EC

Confidence	Economic Capital			Total (Undiversified) EC		Total Diversified EC	Diversification
	Commercial	Retail	Investment	Total Credit	All	All	Benefit
99.00%	726	482	349	1,208	1,557	1,370	12%
99.90%	1,179	741	464	1,920	2,383	2,156	10%
99.99%	1,672	1,003	558	2,674	3,232	2,971	8%

The diversification benefits are calculated by comparing the diversified with the undiversified EC.

7. Benchmark with Other Approaches (Example II)

We now benchmark our calculations with some other approaches.

7.1. Kendall's Tau

Kendall's tau can be used to estimate θ . It is defined for any two random variables X and Y (and their independent copy (X^*, Y^*)) as

$$\tau(X, Y) = Prob\{(X - X^*)(Y - Y^*) > 0\} - P\{(X - X^*)(Y - Y^*) < 0\}.$$

We estimate θ between the Fed's C&I and retail charge-offs through our formula (Proposition 5.2) and Kendall's tau (see Table 6).

Table 6

Benchmark θ

Fed C&I and Retail CO	Estimation of θ
Ours	1.4068
Kendall's tau	1.4541

7.2. EC under the Nested Copula Method

The Nested Copula approach breaks the calculation of a multidimensional copula into a series of two-dimensional fittings. In our three-portfolio case, we choose to first aggregate two credit portfolios, and the outcome is then aggregated with the investment portfolio. Here is the procedure:

- 1) *Generate uniform distributions from Fed and S&P500 data through percentile ranking*
- 2) *Calculate the interim parameter θ between C&I and retail portfolios using either Kendall's tau or Proposition 5.2*
- 3) *Simulate the interim copula to aggregate credit portfolio losses*
- 4) *Generate a uniform distribution for the interim copula; to be able to incorporate the historical data, the interim copula has to be generated in a way that is consistent with the observed percentile ranks*
- 5) *Calculate the final parameter θ between the interim copula and the investment portfolio using either Kendall's tau or Proposition 5.2*
- 6) *Simulate the final copula*
- 7) *Apply the simulated copula to the simulated interim loss distribution and the investment portfolio loss distribution to derive the aggregated (diversified) EC.*

Table 7 summarizes our benchmarking results.

Table 7**Nested Copula Approach**

Nested Copula			
Interim θ	Undiversified	Diversified	Diversification
1.4068	Credit Portfolio EC	Interim Portfolio EC	Benefit
99.00%	1,208	1,084	10%
99.90%	1,920	1,776	8%
99.99%	2,674	2,506	6%
Nested Copula			
Final θ	Undiversified	Diversified	Diversification
1.1772	Total EC	Total EC	Benefit
99.00%	1,557	1,347	13%
99.90%	2,383	2,138	10%
99.99%	3,232	2,922	10%

The results are compared with our calculations in Example I in Table 8.

Table 8**Benchmark EC**

\$mm	Undiversified	Our Approach	Nested Copula
Confidence	Total EC	Total EC	Total EC
99.00%	1,557	1,370	1,347
99.90%	2,383	2,156	2,138
99.99%	3,232	2,971	2,922

8. Closing Notes

The parameter θ of a multidimensional Gumbel copula can be estimated directly through the roots of a polynomial. We demonstrated its application in aggregating the EC of typical bank portfolios. When benchmarked with the Nested Copula approach, it avoids all interim calibrations and calculations that have to be performed using sophisticated techniques to maintain consistency with the observed data.

Appendix A: Proof of Our Results

In the appendix we provide a proof for our formulae in Proposition 5.2.

1. $K(t)$ is a polynomial of degree $k - 1$ in z for $z = \frac{1}{\theta}$.

Proof: Since $K(t) = t + \sum_{i=1}^{k-1} (-1)^i \frac{\{\phi(t)\}^i}{i!} \frac{d^i}{dx^i} \phi^{-1}(x) \Big|_{x=\phi(t)}$ with $\phi(t) = (-\ln t)^\theta$ and

$t = \phi^{-1}(x) = e^{-x^{\frac{1}{\theta}}}$, we calculate the following:

$$\frac{d}{dx} \phi^{-1}(x) = e^{-x^{\frac{1}{\theta}}} \left(-\frac{1}{\theta} x^{\frac{1}{\theta}-1} \right) = e^{-x^{\frac{1}{\theta}}} \left(-\frac{1}{\theta} \frac{x^{\frac{1}{\theta}}}{x} \right) = -\frac{1}{\theta} e^{-x^{\frac{1}{\theta}}} \frac{x^{\frac{1}{\theta}}}{x} = -\frac{1}{\theta} t \frac{-\ln t}{x} = zt \frac{\ln t}{x}.$$

Therefore

$$\phi(t) \frac{d}{dx} \phi^{-1}(x) \Big|_{x=\phi(t)} = x \frac{d}{dx} \phi^{-1}(x) = zt \ln t.$$

In particular, $\frac{dt}{dx} = \frac{d}{dx} \phi^{-1}(x) = \frac{zt \ln t}{x}$.

Assume inductively $\{\phi(t)\}^i \frac{d^i}{dx^i} \phi^{-1}(x) \Big|_{x=\phi(t)} = t \sum_{j=1}^i Q_j^i \cdot \ln^j t$, then we have

$$\begin{aligned} \frac{d}{dx} \left(\{\phi(t)\}^i \frac{d^i}{dx^i} \phi^{-1}(x) \right) &= \frac{d}{dx} \left(x^i \frac{d^i}{dx^i} \phi^{-1}(x) \right) = ix^{i-1} \frac{d^i}{dx^i} \phi^{-1}(x) + x^i \frac{d^{i+1}}{dx^{i+1}} \phi^{-1}(x) \\ &= \frac{d}{dx} \left(t \sum_{j=1}^i Q_j^i \cdot \ln^j t \right) = \frac{d}{dt} \left(t \sum_{j=1}^i Q_j^i \cdot \ln^j t \right) \cdot \frac{dt}{dx} = \left(\sum_{j=1}^i Q_j^i \cdot \ln^j t + t \sum_{j=1}^i Q_j^i \cdot j \cdot \frac{\ln^{j-1} t}{t} \right) \cdot \frac{zt \ln t}{x} \\ &= \left(\sum_{j=1}^i Q_j^i \cdot \ln^j t + \sum_{j=1}^i Q_j^i \cdot j \cdot \ln^{j-1} t \right) \cdot \frac{zt \ln t}{x} = \frac{zt}{x} \left(\sum_{j=2}^{i+1} Q_{j-1}^i \cdot \ln^j t + \sum_{j=1}^i Q_j^i \cdot j \cdot \ln^j t \right) \end{aligned}$$

$$= \frac{t}{x} \left(\sum_{j=1}^{i+1} z(Q_{j-1}^i + Q_j^i \cdot j) \cdot \ln^j t \right) \text{ with } Q_j^i = 0 \text{ for } j > i \text{ or } j \leq 0.$$

Hence

$$\begin{aligned} x^{i+1} \frac{d^{i+1}}{dx^{i+1}} \phi^{-1}(x) &= x \cdot \left(\frac{t}{x} \left(\sum_{j=1}^{i+1} z(Q_{j-1}^i + Q_j^i \cdot j) \cdot \ln^j t \right) - ix^{i-1} \frac{d^i}{dx^i} \phi^{-1}(x) \right) \\ &= t \left(\sum_{j=1}^{i+1} z(Q_{j-1}^i + Q_j^i \cdot j) \cdot \ln^j t \right) - ix^i \frac{d^i}{dx^i} \phi^{-1}(x) = t \left(\sum_{j=1}^{i+1} z(Q_{j-1}^i + Q_j^i \cdot j) \cdot \ln^j t \right) - i \cdot t \sum_{j=1}^i Q_j^i \cdot \ln^j t \\ &= t \left(\sum_{j=1}^{i+1} (zQ_{j-1}^i + (z \cdot j - i) \cdot Q_j^i) \cdot \ln^j t \right) = t \left(\sum_{j=1}^{i+1} Q_j^{i+1} \cdot \ln^j t \right) \end{aligned}$$

$$\text{for } Q_j^{i+1} = zQ_{j-1}^i + (z \cdot j - i) \cdot Q_j^i.$$

2. For $k = 2$, we have $K(t) = t - \phi(t) \frac{d}{dx} \phi^{-1}(x) \Big|_{x=\phi(t)} = t - zt \ln t$.

Proof: First, we calculate, for any constant c , the indefinite integral

$$\begin{aligned} \int (K(t) - c)^2 dt &= \int (t - zt \ln t - c)^2 dt \\ &= \left(\frac{2}{27} - \frac{2 \ln t}{9} + \frac{\ln^2 t}{3} \right) t^3 z^2 + \left(\frac{2t^3}{9} - \frac{ct^2}{2} + ct^2 \ln t - \frac{2t^3 \ln t}{3} \right) z + \left(\frac{t^3}{3} - ct^2 + c^2 t \right). \end{aligned}$$

$$\begin{aligned} \text{Hence } \int_0^1 (K(t) - \hat{K}(t))^2 dt &= \int_0^{w_1^*} (K(t) - \hat{K}(t))^2 dt + \sum_{i=1}^{Q-1} \int_{w_i^*}^{w_{i+1}^*} (K(t) - \hat{K}(t))^2 dt + \int_{w_Q^*}^1 (K(t) - \hat{K}(t))^2 dt \\ &= \int_0^{w_1^*} (K(t))^2 dt + \sum_{i=1}^{Q-1} \int_{w_i^*}^{w_{i+1}^*} (K(t) - k_i)^2 dt + \int_{w_Q^*}^1 (K(t) - k_Q)^2 dt = \frac{2}{27} z^2 + \alpha \cdot z + \omega \end{aligned}$$

$$\text{for } \alpha = \frac{2}{9} + \sum_{i=1}^Q k_i \left\{ \left(\ln w_{i+1}^* - \frac{1}{2} \right) w_{i+1}^{*2} - \left(\ln w_i^* - \frac{1}{2} \right) w_i^{*2} \right\} \text{ and } \omega = \frac{1}{3} + \sum_{i=1}^Q \left\{ k_i^2 (w_{i+1}^* - w_i^*) - k_i (w_{i+1}^2 - w_i^2) \right\}.$$

This quadratic equation reaches its minimal when $z = -\frac{27}{4}\alpha$ or $\theta = -\frac{4}{27\alpha}$.

3. For $k=3$, we have $K(t) = t + t \ln t \left(\frac{z^2 - 3z}{2} \right) + t \ln^2 t \frac{z^2}{2}$.

Proof: Similarly, we calculate following integrals assuming $k_0 = 0$, $w_0^* = 0$, and $w_{Q+1}^* = 1$,

$$\int_0^1 K^2(t) dt = \frac{1}{3} + \frac{1}{3}z + \frac{7}{54}z^2 + \frac{1}{164}z^4, \text{ and}$$

$$\int K(t) dt = \frac{t^2}{2} + \left(\frac{3t^2}{8} - \frac{3t^2 \ln t}{4} \right) z + \frac{t^2 \ln^2 t}{4} z^2.$$

$$\begin{aligned} \text{Therefore } \int_0^1 \left(K(t) - \hat{K}(t) \right)^2 dt &= \int_0^1 K^2(t) dt - 2 \int_0^1 K(t) \cdot \hat{K}(t) dt + \int_0^1 \hat{K}^2(t) dt \\ &= \frac{1}{3} + \frac{1}{3}z + \frac{7}{54}z^2 + \frac{1}{164}z^4 - 2 \int_0^1 K(t) \cdot \hat{K}(t) dt + \int_0^1 \hat{K}^2(t) dt \\ &= \frac{1}{3} + \frac{1}{3}z + \frac{7}{54}z^2 + \frac{1}{164}z^4 - 2 \sum_{i=0}^Q \int_{w_i^*}^{w_{i+1}^*} K(t) \cdot \hat{K}(t) dt + \int_0^1 \hat{K}^2(t) dt \\ &= \frac{1}{3} + \frac{1}{3}z + \frac{7}{54}z^2 + \frac{1}{164}z^4 - 2 \sum_{i=0}^Q \int_{w_i^*}^{w_{i+1}^*} K(t) \cdot \hat{K}(t) dt + \sum_{i=0}^Q \int_{w_i^*}^{w_{i+1}^*} \hat{K}^2(t) dt \\ &= \frac{1}{3} + \frac{1}{3}z + \frac{7}{54}z^2 + \frac{1}{164}z^4 - 2 \sum_{i=0}^Q \int_{w_i^*}^{w_{i+1}^*} K(t) \cdot k_i dt + \sum_{i=0}^Q \int_{w_i^*}^{w_{i+1}^*} k_i^2 dt \\ &= \frac{1}{3} + \frac{1}{3}z + \frac{7}{54}z^2 + \frac{1}{164}z^4 - 2 \sum_{i=0}^Q k_i \cdot \int_{w_i^*}^{w_{i+1}^*} K(t) dt + \sum_{i=0}^Q k_i^2 (w_{i+1}^* - w_i^*) \end{aligned}$$

$$\begin{aligned}
&= \frac{1}{3} + \frac{1}{3}z + \frac{7}{54}z^2 + \frac{1}{164}z^4 + \sum_{i=0}^Q k_i^2 (w_{i+1}^* - w_i^*) + \\
&- 2 \sum_{i=0}^Q k_i \cdot \left\{ \left(\frac{w_{i+1}^{*2} - w_i^{*2}}{2} + \left(\frac{3 \cdot (w_{i+1}^{*2} - w_i^{*2})}{8} - \frac{3 \cdot (w_{i+1}^{*2} \ln w_{i+1}^* - w_i^{*2} \ln w_i^*)}{4} \right) z + \frac{(w_{i+1}^{*2} \ln^2 w_{i+1}^* - w_i^{*2} \ln^2 w_i^*)}{4} z^2 \right) \right\} \\
&= \frac{1}{164}z^4 + \left(\frac{7}{54} - \sum_{i=0}^Q k_i \cdot \frac{(w_{i+1}^{*2} \ln^2 w_{i+1}^* - w_i^{*2} \ln^2 w_i^*)}{2} \right) z^2 \\
&+ \left(\frac{1}{3} - 2 \sum_{i=0}^Q k_i \cdot \left(\frac{3 \cdot (w_{i+1}^{*2} - w_i^{*2})}{8} - \frac{3 \cdot (w_{i+1}^{*2} \ln w_{i+1}^* - w_i^{*2} \ln w_i^*)}{4} \right) \right) z + \sum_{i=0}^Q k_i^2 (w_{i+1}^* - w_i^*) + \frac{1}{3}.
\end{aligned}$$

This is a polynomial of degree 4. Its minimal will be reached at the roots of its derivative polynomial:

$$\frac{2}{81}z^3 + \left(\frac{7}{27} - \sum_{i=0}^Q k_i \cdot (w_{i+1}^{*2} \ln^2 w_{i+1}^* - w_i^{*2} \ln^2 w_i^*) \right) z + \left(\frac{1}{3} + \sum_{i=0}^Q k_i \cdot \left(\frac{3 \cdot (w_{i+1}^{*2} \ln w_{i+1}^* - w_i^{*2} \ln w_i^*)}{2} - \frac{3 \cdot (w_{i+1}^{*2} - w_i^{*2})}{4} \right) \right).$$

Since this polynomial is of degree 3 without a degree 2 term, its positive real root is

$$z = \sqrt[3]{-\frac{81\gamma}{4} + \sqrt{\frac{6561\gamma^2}{16} + \frac{19683\beta^3}{8}}} + \sqrt[3]{-\frac{81\gamma}{4} - \sqrt{\frac{6561\gamma^2}{16} + \frac{19683\beta^3}{8}}} \text{ with}$$

$$\beta = \frac{7}{27} - \sum_{i=1}^Q k_i \{w_{i+1}^{*2} \ln^2 w_{i+1}^* - w_i^{*2} \ln^2 w_i^*\}; \text{ and}$$

$$\gamma = \frac{1}{3} + \sum_{i=1}^Q k_i \left\{ \frac{3}{2} (w_{i+1}^{*2} \ln w_{i+1}^* - w_i^{*2} \ln w_i^*) - \frac{3}{4} (w_{i+1}^{*2} - w_i^{*2}) \right\}.$$

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